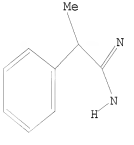
7 8 9 12
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
10 11
chain bonds :
5-7 7-8 7-9 9-10 9-11 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
9-10 9-11
exact bonds :
5-7 7-8 7-9 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 10:41:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 360 TO ITERATE

100.0% PROCESSED 360 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 6062 TO 8338

PROJECTED ANSWERS: 9 TO 360

L2 9 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:41:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6833 TO ITERATE

100.0% PROCESSED 6833 ITERATIONS 137 ANSWERS
SEARCH TIME: 00.00.01

L3 137 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 178.36 178.57

FILE 'CAPLUS' ENTERED AT 10:41:42 ON 05 JUN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 5 Jun 2008 VOL 148 ISS 23
FILE LAST UPDATED: 4 Jun 2008 (20080604/ED)

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They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l3
L4 60 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1303013 CAPLUS
DOCUMENT NUMBER: 147:541746
TITLE: Preparation of quinolinones and analogs as antiviral agents
INVENTOR(S): Kumar, Dange V.; Rai, Roopa; Young, Wendy B.; Hu, Huiyong; Riggs, Jennifer R.; Ton, Tony Loc; Green, Michael J.; Hart, Barry P.; Brameld, Kenneth A.; Dener, Jeff M.
PATENT ASSIGNEE(S): Virobay, Inc., USA
SOURCE: PCT Int. Appl., 201pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007130499	A2	20071115	WO 2007-US10702	20070430
WO 2007130499	A3	20080110		

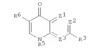
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070287699	A1	20071213	US 2007-742461	20070430
PRIORITY APPLN. INFO.:			US 2006-796943P P	20060501

OTHER SOURCE(S): MARPAT 147:541746
GI

L4 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)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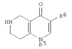
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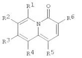
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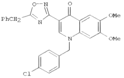
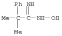

IV

AB Title compds. represented by the formula I & II & III [wherein Z1 = N or CR1; Z2 = N or CR2; Z3 = N or CR4; R1 = H, halo, alkyl, etc.; R2 = H, halo, alkoxy, etc.; R3 = halo, alkyl, aryl, etc.; R4 = H, halo, haloalkyl, etc.; R5 = alkyl, cycloalkylamino, arylamino, etc.; R6 = (un)substituted 1,2,4-oxadiazol-3-yl, 1,2,4-oxadiazol-5-yl, 1,3,4-oxadiazol-2-yl or oxazol-2-yl; and pharmaceutically acceptable salts thereof] were prepared as antiviral agents. For example, IV was provided in a multi-step synthesis starting from reaction of Et 2-cyano-3-ethoxyacrylate with 3,4-dimethoxyphenylamine. The invention compds. showed activity in HCV replicon assays and their formulations were also presented. Thus, the title compds. and their pharmaceutical compns. are useful for the treatment of viral infections, particularly HCV.

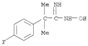
IT 957140-71-5, N-Hydroxy-2-methyl-2-phenylpropanimidamide
957140-73-7, 2-(4-Fluorophenyl)-N-hydroxy-2-methylpropanimidamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-quinolinones and analogs as antiviral agents)

RN 957140-71-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α,α-dimethyl- (CA INDEX NAME)

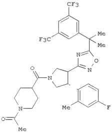


RN 957140-73-7 CAPLUS

L4 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CN Benzeneethanimidamide, 4-fluoro-N-hydroxy-α,α-dimethyl- (CA INDEX NAME)



L4 ANSWER 2 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1050755 CAPLUS
DOCUMENT NUMBER: 148:385
TITLE: Pyrrolidine-carboxamides and oxadiazoles as potent hNK1 antagonists
AUTHOR(S): Young, Jonathan R.; Eid, Ronsar; Turner, Cherilyn; DeVita, Robert J.; Kurtz, Marc M.; Tsao, Kwei-Lan C.; Chicchi, Gary G.; Wheeldon, Alan; Carlson, Emma; Mills, Sander G.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065-0900, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(19), 5310-5315
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI


I

AB The preparation and structure-activity relationships of novel pyrrolidine-carboxamides and oxadiazoles are described. Compds. in this series were found to be potent hNK1 antagonists in vitro and efficacious in vivo with minimal interactions with P450 liver enzymes. Oxadiazole analog (I) was determined to have excellent hNK1 binding affinity, functional activity, and a good PD response in vivo.

IT 957476-30-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(pyrrolidine-carboxamides and oxadiazoles as potent hNK1 antagonists)

RN 957476-30-1 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α,α-dimethyl-3,5-bis(trifluoromethyl)- (CA INDEX NAME)

L4 ANSWER 2 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:744613 CAPLUS
DOCUMENT NUMBER: 146:454167
TITLE: 6-alkylthio-4-(1-(2,6-difluorophenyl)alkyl)-1H-[1,2,5]triazin-2-ones (DATs): novel regulators of cell differentiation and proliferation
AUTHOR(S): Skardelis, Gianluca; Bartolini, Sara; Castellano, Sabrina; Artico, Marino; Fermeno, Nicola; Rotili, Dante; Spadafora, Corrado; Ma, Antonello
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita degli Studi di Salerno, Fisciano, 84084, Italy
SOURCE: ChemMedChem (2006), 1(10), 1073-1080
CODEN: CHEMKG; ISSN: 1860-7179
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:454167
GI

I

AB Novel triazine analogs of 5-alkyl-2-alkylthio-6-(1-(2,6-difluorophenyl)alkyl)-3,4-dihydropyrimidin-4(3H)-ones (F2-DABOs), previously described by us as nonnucleoside HIV-1 reverse transcriptase inhibitors (NNRTIs), were tested for their antiproliferative and cytodifferentiating activity on the A-375 human melanoma cell line. Most of the tested deriv. were effective in decreasing cell proliferation, facilitating morphol. differentiation, and reprogramming gene expression. All these effects were reversable upon withdrawal of PZ inhibitors. Among the compds. tested, 3f (I) showed the highest antiproliferative effect, whereas compound 6c, although not affecting cell proliferation, is endowed with a strong cytodifferentiating effect, which is probably related to a marked upregulation of the n-cad gene. These results support the potential of NNRTIs as valuable antitumor agents.
IT 935480-63-0P
RLs: BCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(triazinones as regulators of cell differentiation and proliferation)

L4 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 935480-63-0 CAPLUS
CN Benzenemethanimidamide, 2,6-difluoro-4-methyl- (CA INDEX NAME)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:174606 CAPLUS
DOCUMENT NUMBER: 146:251662
TITLE: Xanthine derivatives as selective HM74A agonists and their preparation
INVENTOR(S): Bailey, Richard Jonathan Daniel; Heer, Jag Paul; Liddle, John; Mason, Andrew Nemurtrie; Panto, Ivan Lee; Rahman, Shahzad Sharoogy Smith, Ian Edward David
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 312pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007017262	A1	20070215	WO 2006-EP7869	20060808
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006278216	A1	20070215	AU 2006-278216	20060808
CA 2618963	A1	20070215	CA 2006-2618963	20060808
EP 1922892	A1	20080523	EP 2006-776699	20060808
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
KR 2008039394	A	20080506	KR 2008-705724	20080307
PRIORITY APPLN. INFO.:			GB 2005-16464	A 20050810
			GB 2006-7736	A 20060419
			GB 2006-14569	A 20060721
			WO 2006-EP7869	W 20060808

OTHER SOURCE(S): MARPAT 146:251662
GI

L4 ANSWER 4 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

AB The invention relates to compds. of formula I, which are xanthine derivs., processes for the manufacture of said derivs., pharmaceutical formulations containing the active compds. and the use of the compds. in therapy, for example, in the treatment of diseases where under-activation of the HM74A receptor contributes to the disease or where activation of the receptor will be beneficial. Compds. of formula I wherein R1 is (un)substituted C1-5 alkylene; R2 is H, (un)substituted C1-10 alkyl, (un)substituted C2-10 alkenyl, (un)substituted C2-10 alkynyl, (un)substituted cycloalkyl, (un)substituted cycloalkenyl, (un)substituted heterocyclyl, and (un)substituted heteroaryl; R3 is halo and CN; and their pharmaceutically acceptable deriv. thereof, are claimed. Example compound II was prepared by alkylation of 8-chloro-3-pentyl-7-[2-propen-1-yl]-3,7-dihydro-1H-purine-2,6-dione with 2-chlorowethanol followed by dealkylation. All the invention compds. were evaluated for their HM74A agonistic activity.

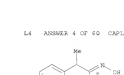
IT 925444-91-7P 925444-93-0P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of xanthine derivs. as selective HM74A agonists)

RN 925444-91-7 CAPLUS
CN Benzeneethaninidamide, 3-bromo-N-hydroxy-α,α-dimethyl-, [C(Z)]- (CA INDEX NAME)

Double bond geometry as shown.

RN 925444-98-0 CAPLUS
CN Benzeneethaninidamide, N,4-dihydroxy-α,α-dimethyl-, [C(Z)]-

L4 ANSWER 4 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● RC1

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(CA INDEX NAME)

Double bond geometry as shown.

IT 62191-51-5 925698-75-5 925893-03-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of xanthine deriv. as selective HM74A agonists)

RN 62191-51-5 CAPLUS
CN Benzeneethaninidamide, N-hydroxy-α-methyl- (CA INDEX NAME)

RN 925698-75-5 CAPLUS
CN Benzeneethaninidamide, N-hydroxy-α-methyl-, [C(Z)]- (CA INDEX NAME)

Double bond geometry as shown.

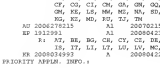
RN 925893-03-4 CAPLUS
CN Benzeneethaninidamide, 4-chloro-N-hydroxy-α-methyl-, hydrochloride
(1:1) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 5 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:176405 CAPLUS
DOCUMENT NUMBER: 146:251661
TITLE: Preparation of xanthine derivatives as selective HM74A agonists
INVENTOR(S): Hatley, Richard Jonathan Daniel; Mason, Andrew Nomuritis; Pinto, Ivan Leo
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 109pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

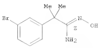
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007017261	A1	20070215	WO 2006-EP7865	20060808
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2006278215	A1	20070215	AU 2006-278215	20060808
EP 1912991	A1	20080423	EP 2006-763016	20060808
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF				
KR 20080034992	A	20080422	KR 2008-701717	20080207
PRIORITY APPLN. INFO.:			GB 2005-16464	A 20050810
			GB 2006-7736	A 20060419
			GB 2006-14569	A 20060721
			WO 2006-EP7865	W 20060808

OTHER SOURCE(S): MARPAT 146:251661
GI



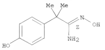
L4 ANSWER 5 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
AB Xanthine derivs. of formula I [R1 = (CH2)mX(CH2)nY; X = heteroaryl, heterocyclyl; Y = (substituted) aryl, heteroaryl, aryloxy; m = 3-4; n = 0-1; R2 = (substituted) alkyl; R3 = halo] are prepared for the treatment of diseases where under-activation of the HM74A receptor contributes to the disease or where activation of the receptor will be beneficial. Thus, II was prepared from 3-pentyl-8-chloro-7-allyl-3,7-dihydro-1H-purine-2,6-dione, 4-(3-hydroxypropyl)pyrazole and 2-chloro-6-fluorobenzyl bromide. The prepared compds. had pEC50 values ≥ 4.3 and efficacy ≥ 30% in GTPγS binding assays.
IT 925444-91-3P 925444-98-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of xanthine derivs. as selective HM74A agonists)
RN 925444-91-3 CAPLUS
CN Benzeneethanimidamide, 3-bromo-N-hydroxy-α,α-dimethyl-, [C(Z)]- (CA INDEX NAME)

Double bond geometry as shown.



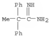
RN 925444-98-0 CAPLUS
CN Benzeneethanimidamide, N,4-dihydroxy-α,α-dimethyl-, [C(Z)]- (CA INDEX NAME)

Double bond geometry as shown.



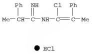
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:30368 CAPLUS
DOCUMENT NUMBER: 146:317014
TITLE: New Optically Active N-Heterocyclic Carbene Complexes for Hydrogenation: A Tale with an Atropisomeric Twist
AUTHOR(S): Chen, Dianjun; Banphavichit, Vorawit; Reibenspies, Joe; Burgess, Kevin
CORPORATE SOURCE: Department of Chemistry, Texas A and M University, College Station, TX, 77843, USA
SOURCE: Organometallics (2007), 26(4), 855-859
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:317014
AB Iridium chiral 1,2,4-triazol-3-ylidene pyrimidine complexes derived from isoleucine were prepared and examined as catalysts for asym. hydrogenation of 1,2-diphenyl-1-propene; the complexes low enantioselectivity of 12% ee. Homologation and alkynylation of L-isoleucine afforded (3S,4R)-4-Boc-amino-3-methyl-7-dodecyn-6-one (8), which was condensed with amidines R(:NH)NH2 to give N-Boc-protected (αR)-2-R-6-Bu-α-[(1S)-1-methylpropyl]-4-pyrimidineethanamines (9a-c; R = Ph, 1-adamantyl, CMePh2). Deprotection of 9a-c followed by reaction with 3-(1-adamantyl)-1,3,4-oxadiazolium tetrafluoroborate gave the ligand precursors, 1-adamantyl-4-[(1R,2S)-1-(2-R-6-butyl-4-pyrimidinylmethyl)-2-methylbutyl]tetrazolium tetrafluoroborates (2a-c; R = Ph, 1-adamantyl, CMePh2), which upon metalation and halogen abstraction afforded the corresponding cationic iridium carbene-pyrimidine chelate cyclooctadiene complexes (5). A structure of the 1,2,4-triazolium salts is easily varied, allowing an access to a diverse set of N-heterocyclic carbene complexes. A coordinated chlorine atom was retained on reaction of 2 with [Ir(COD)Cl]2, and this resulted in two atropoisomeric complexes, 3 and 4, which were both characterized via x-ray diffraction studies. Neither of these complexes mediated hydrogenation of (E)-1,2-diphenyl-1-propene, but both 3 and 4 were reacted with NaBArF4 to give the chlorine-free complex 5, which was catalytically active in this reaction.
IT 173601-37-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chiral carbene iridium triazolylidene-pyrimidine chelate complexes as catalysts for asym. hydrogenation of alkenes)
RN 173601-37-1 CAPLUS
CN Benzeneethanimidamide, α-methyl-α-phenyl- (CA INDEX NAME)



L4 ANSWER 6 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:189333 CAPLUS
DOCUMENT NUMBER: 146:228672
TITLE: Product subclass 4: 1-nitrogen-functionalized 1-haloalk-1-enes
AUTHOR(S): Schantl, J. G.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2006), Volume Date 2005, 24, 223-284
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of methods to prepare 1-nitrogen-functionalized 1-haloalk-1-enes.
IT 40645-76-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(review preparation of nitrogen functionalized haloalkenes)
RN 40645-76-9 CAPLUS
CN Benzeneethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



REFERENCE COUNT: 154 THERE ARE 154 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:351699 CAPLUS
DOCUMENT NUMBER: 144:467615
TITLE: Amidines (imidamidal) N-substituted by metals, halogens, oxygen, and other heteroatoms
AUTHOR(S): Ostrowska, K.; Kolasa, A.
CORPORATE SOURCE: Warsaw
SOURCE: Science of Synthesis (2005), 22, 489-563
CODEN: SSCYIS
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of the preparation and synthetic applications of amidine derivs.
IT 140154-96-5D
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and synthetic applications of amidine derivs.)
RN 140154-96-5 CAPLUS
CN Benzeneethanimidic acid, a-hydroxy-a-methyl-, hydrazide (CA INDEX NAME)

REFERENCE COUNT: 939 THERE ARE 939 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:287457 CAPLUS
DOCUMENT NUMBER: 142:355052
TITLE: Preparation of amidines and their salts useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8
INVENTOR(S): Allegretti, Marcello; Cesta, Maria Candida; Nano, Giuseppe; Bertini, Riccardo; Bizzarri, Cinzia; Colotta, Francesco
PATENT ASSIGNEE(S): Dompe S.P.A., Italy
SOURCE: PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005028425	A2	20050331	WO 2004-EP52201	20040916
WO 2005028425	A3	20050609		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004274183	A1	20050331	AU 2004-274183	20040916
CA 2539842	A1	20050331	CA 2004-2539842	20040916
EP 1663960	A2	20060607	EP 2004-787150	20040916
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1882526	A	20061220	CN 2004-80035936	20040916
JP 2007506706	T	20070322	JP 2006-527406	20040916
US 20070185167	A1	20070705	US 2006-568760	20060201
NO 20060001721	A	20060419	NO 2006-1721	20060419
PRIORITY APPLN. INFO.:			EP 2003-103557	A 20030925
			WO 2004-EP52201	W 20040916

OTHER SOURCE(S): CASREACT 142:355052; MARPAT 142:355052
AB Amidines ACH(CH3)C(:NH):NHR1 [A = (un)substituted Ph; benzyl, (un)substituted heteroaryl; R = H, C1-5 alkyl, phenylalkyl, alkenyl, cycloalkyl, alkoxy, etc.; R1 = H, Me, Et; e.g., (R,S)-2-(4-isobutylphenyl)propionamidine hydrochloride], useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8 in the treatment of psoriasis, ulcerative colitis, melanoma, chronic obstructive pulmonary disease, bullous pemphigo, rheumatoid arthritis, idiopathic fibrosis, glomerulonephritis, and in the prevention and treatment of damages caused by ischemia and reperfusion., are prepared
IT 261178-48-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in the preparation of amidines and their salts useful in the inhibition of

L4 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:203457 CAPLUS
DOCUMENT NUMBER: 143:326018
TITLE: Synthesis and biological activity of flurbiprofen analogues as selective inhibitors of β-amyloid(1-42) secretion
AUTHOR(S): Peretto, Ilaria; Radaelli, Stefano; Parini, Carlo; Zandi, Michele; Savoldia, Luca F.; Bordio, Giulio; Fontanella, Luca; Rizzano, Paola; Scapozza, Chiara; Rizzi, Andrea; Riccardi, Benedetta; Biscoldi, Marcello; Marchetti, Silvia; Patrini, Paolo; Catanella, Silvia; Bondelli, Ivano; Cenacchi, Valentina; Bolognesi, Maria Laura; Perini, Paolo; Villetti, Gino; Facchinetti, Fabrizio; Del Giudice, Elda; Moretti, Nadia; Imbimbo, Bruno P.
CORPORATE SOURCE: Research Development, Chiesi Farmaceutici S.p.A., Parma, 43100, Italy
SOURCE: Journal of Medicinal Chemistry (2005), 48(10), 5705-5720
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:326018
AB Flurbiprofen, a nonsteroidal antiinflammatory drug (NSAID), was recently described to selectively inhibit β-amyloid-42 (Aβ42) secretion, the most toxic component of the senile plaques present in the brain of Alzheimer patients. The use of this NSAID in Alzheimer's disease (AD) is hampered by a significant gastrointestinal toxicity associated with cyclooxygenase (COX) inhibition. New flurbiprofen analogs were synthesized, with the aim of increasing Aβ42 inhibitory potency while removing anti-COX activity. In vitro ADME developability parameters were taken into account in order to identify optimized compds. at an early stage of the project. Appropriate substitution patterns at the alpha position of flurbiprofen allowed for the complete removal of anti-COX activity, while modifications at the terminal Ph ring resulted in increased inhibitory potency on Aβ42 secretion. In fact, some of the compds. appeared to be well absorbed after oral administration and to penetrate into the central nervous system. Studies in a transgenic mice model of AD showed that selected compds. significantly decreased plasma Aβ42 concns. These new flurbiprofen analogs represent potential drug candidates to be developed for the treatment of AD.
IT 884925-31-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. activity of flurbiprofen analogs as selective inhibitors of β-amyloid(1-42) secretion devoid of anti-cyclooxygenase activity)
RN 884925-31-1 CAPLUS
CN [1,1'-Biphenyl]-4-ethanimidamide, 2-fluoro-N-hydroxy-α-methyl-4'-(trifluoromethyl)- (CA INDEX NAME)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
chemotaxis of neutrophils induced by interleukin-8)
RN 261178-48-7 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(2-methylpropyl)- (CA INDEX NAME)

IT 849063-66-7P 849063-67-8P
RL: PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidines and their salts useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8)
RN 849063-66-7 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, (+)- (CA INDEX NAME)

Rotation (+).

RN 849063-67-8 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, (-)- (CA INDEX NAME)

Rotation (-).

IT 849063-49-6P 849063-50-9P 849063-51-0P
849063-52-1P 849063-53-2P 849063-54-3P
849063-56-5P 849063-57-6P 849063-58-7P
849063-59-8P 849063-60-1P 849063-61-2P

L4 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

● HCl

RN 849063-52-1 CAPLUS
CN Benzeneethanimidamide, 3-benzoyl-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 849063-53-2 CAPLUS
CN 1,3,5-Benzenetriacetamidine, 2-fluoro-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 849063-54-3 CAPLUS
CN Methanesulfonic acid, 1,1,1-trifluoro-, 4-(2-amino-2-imino-1-methylethyl)phenyl ester, hydrochloride (1:1) (CA INDEX NAME)

L4 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidines and their salts useful in the inhibition of chemotaxis of neutrophils induced by interleukin-8)
RN 849063-49-6 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 849063-50-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, hydrochloride (1:1), (+)- (CA INDEX NAME)

Rotation (+).

● HCl

RN 849063-51-0 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, hydrochloride (1:1), (-)- (CA INDEX NAME)

Rotation (-).

L4 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

● HCl

RN 849063-56-5 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-N-[3-(1-piperidinyl)propyl]-, hydrochloride (1:2) (CA INDEX NAME)

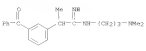
● 2 HCl

RN 849063-57-6 CAPLUS
CN Benzeneethanimidamide, N,α-dimethyl-4-(2-methylpropyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 849063-58-7 CAPLUS
CN Benzeneethanimidamide, 3-benzoyl-N-[3-(dimethylamino)propyl]-α-methyl-, hydrochloride (1:2) (CA INDEX NAME)

L4 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

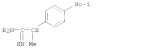


● 2 HCl

RN 849063-59-8 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-, acetate (1:1) (CA INDEX NAME)

CM 1

CRN 487067-20-5
CMF C13 H20 N2

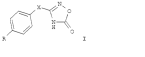


CM 2

CRN 64-19-7
CMF C2 H4 O2

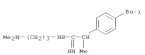
RN 849063-60-3 CAPLUS
CN Benzeneethanimidamide, N-[3-(dimethylamino)propyl]-α-methyl-4-(2-methylpropyl)- (CA INDEX NAME)

L4 ANSWER 11 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:150232 CAPLUS
DOCUMENT NUMBER: 142:413301
TITLE: Inhibition of secretory phospholipase A2. 2-Synthesis and structure-activity relationship studies of 4,5-dihydro-5-(4-tetradecyloxybenzyl)-1,2,4-oxadiazol-5-one (PMS1062) derivatives specific for group II enzyme
AUTHOR(S): Dong, Chang-Zhi; Ahanada-Hinidi, Azali; Plocki, Stephane; Aoun, Dalia; Touaibia, Mohamed; Meddad-Bel Habich, Nadia; Poet, Jack; Redeuilh, Catherine; Ombetta, Jean-Edouard; Godfrold, Jean-Jacques; Massiot, France; Heynars, Francoise
CORPORATE SOURCE: Unite de Pharmacochimie Moleculaire et Systemes Membranaires (EA2381), Laboratoire de Pharmacochimie Moleculaire, Universite Paris 7-Denis Diderot, Paris, 75251, Fr.
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(6), 1989-2007
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:413301
GI

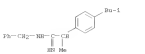


AB The discovery of a series of specific inhibitors of human group IIA phospholipase A2 (hGIIA PLA2) displaying promising in vitro and in vivo properties has been recently reported. Here the influence of different structural modifications on the specificity and potency of oxadiazolones, e.g. 2 (A = CH2, CH2CH2, CHMe, CMe2; X = MeO, n-octyloxy, n-tetradecyloxy, N,N-di(heptyl)amino, etc.), against hGIIA PLA2 vs. porcine group IB PLA2 is described. The SAR results, as well as the log P and pKa values of the oxadiazolones studied provide important information towards the comprehension of the mode of action of this kind of compds.
IT 310869-86-4P 850163-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and calculated hydrophobicity of ether, thioether or amino-functionalized aralkyl oxadiazolones as inhibitors of human secretory phospholipase A2 specific for group II enzyme)
RN 310869-86-4 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(tetradecyloxy)- (CA INDEX NAME)

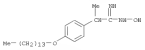
L4 ANSWER 10 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



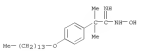
RN 849063-62-2 CAPLUS
CN Benzeneethanimidamide, α-methyl-4-(2-methylpropyl)-N-(phenylmethyl)- (CA INDEX NAME)



L4 ANSWER 11 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 850143-48-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α,α-dimethyl-4-(tetradecyloxy)- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:550957 CAPLUS
DOCUMENT NUMBER: 141:106464
TITLE: Preparation of pyrazolo[3,4-b]pyridine derivatives for use in pharmaceutical compositions as phosphodiesterase inhibitors
INVENTOR(S): Allen, David George; Coe, Diane Mary; Cook, Caroline Mary; Cooper, Anthony William James; Dowle, Michael Dennis; Edlin, Christopher David; Hamblin, Julie Nicole; Johnson, Martin Redpath; Jones, Paul Spencer; Lindvall, Mika Kristian; Mitchell, Charlotte Jane; Redgrave, Alison Judith
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 244 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056823	A1	20040708	WO 2003-EP14867	20031219
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2511340	A1	20040708	CA 2003-2511340	20031219
AU 2003293999	A1	20040714	AU 2003-293999	20031219
EP 1581532	A1	20051005	EP 2003-789413	20031219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017645	A	20051206	BR 2003-17645	20031219
CN 1751042	A	20060322	CN 2003-80109835	20031219
JP 2006513258	T	20060420	JP 2005-502565	20031219
AU 2004299277	A1	20050630	AU 2004-299277	20041217
CA 2557004	A1	20050630	CA 2004-2557004	20041217
WO 2005058892	A1	20050630	WO 2004-EP14490	20041217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1737857	A1	20070103	EP 2004-804089	20041217
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV				
CN 1914205	A	20070214	CN 2004-80041657	20041217
JP 2007514704	T	20070607	JP 2006-544380	20041217
ZA 2005005074	A	20060927	ZA 2005-5074	20050622
IN 2005KN01207	A	20070713	IN 2005-KN1207	20050622
MX 2005PA06923	A	20050818	MX 2005-PA6923	20050623
NO 2005003600	A	20050822	NO 2005-3600	20050722
US 20060252790	A1	20061109	US 2006-540371	20060221
US 20070111995	A1	20070517	US 2006-596561	20060616
IN 2006KN01988	A	20070518	IN 2006-KN1988	20060714
NO 2006003340	A	20060912	NO 2006-3340	20060718

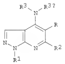
L4 ANSWER 12 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

PRIORITY APPLN. INFO.:

GB 2002-30045	A	20021223
GB 2002-30165	A	20021224
GB 2003-7998	A	20030407
WO 2003-EP14867	W	20031219
WO 2003-EP314867	A	20031219
GB 2004-5899	A	20040316
GB 2004-5936	A	20040316
GB 2004-6754	A	20040325
WO 2004-EP14490	W	20041217

OTHER SOURCE(S): MARPAT 141:106464
GI

L4 ANSWER 12 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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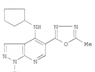
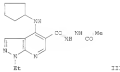


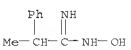
II



III

AB Pyrazolo[3,4-b]pyridine derivs., such as I [R = heterocyclyl; R1 = (CH2)2OH, alkyl, fluoroalkyl; R2 = H, Me, fluoroalkyl; R3 = alkyl, (un)substituted-Ph, cycloalkyl, heterocyclyl, etc.; R3a = H, alkyl], were prepared for therapeutic uses as inhibitors of phosphodiesterase, particularly phosphodiesterase IV (PDE4). These pyrazolo[3,4-b]pyridines were claimed for use in the treatment and/or prophylaxis of cognitive impairment and inflammatory and/or allergic diseases, such as chronic obstructive pulmonary disease (COPD), asthma, or allergic rhinitis. Thus, pyrazolo[3,4-b]pyridine derivative II was prepared via a cyclocondensation reaction of hydrazide III using POCl3 in MeCN. The prepared pyrazolo[3,4-b]pyridine were assayed for PDE4 inhibitory activity, and systems for delivery of these PDE4 inhibitors were discussed.

IT 42191-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolo[3,4-b]pyridine derivs. for use in pharmaceutical compns. as phosphodiesterase inhibitors)
RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

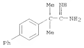
L4 ANSWER 13 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:235774 CAPLUS
DOCUMENT NUMBER: 138:368454
TITLE: Photochemistry of Crystalline Chlorodiazirines: The Influence of Conformational Disorder and Intermolecular Cl···N:N Interactions on the Solid-State Reactivity of Singlet Chlorocarbenes
AUTHOR(S): Sanrame, Carlos N.; Suhrada, Christopher P.; Dang, Hung; Garcia-Garibay, Miguel A.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, 90095-1569, USA
SOURCE: Journal of Physical Chemistry A (2003), 107(18), 3287-3294
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:368454

AB A photochem. study was carried out with 3-R-substituted 3-chlorodiazirines with 4-biphenyl- (4a), (4-biphenyl)methyl- (4b), 2-(4-biphenyl)ethyl- (4c), and 1,1-dimethyl-1-(4-biphenyl)methyl (4d) substituents. The chlorodiazirines were prepared from the corresponding amidines by a procedure involving oxidation with tert-Bu hypochlorite under phase-transfer catalysis. The crystalline nature of 4a-d was established by differential scanning calorimetric anal., which revealed melting endotherms prior to thermal decomposition. Photochem. results in crystalline solids were analogous to those observed in solution, and the products were analyzed in terms of the corresponding singlet-state chlorocarbene intermediates (5a-d). Irradiation of 4a in solution and in crystals resulted in formation of azine RC1C:NN:CC1R 9a (R = C6H4-p-Ph) by reaction of carbene 5a with its precursor. Equally selective, diazirine 4d gave alkene Me2C:CCl(C6H4-p-Ph) 6d as the only product by a 1,2-Ph migration from carbene 5d. In contrast, irradiation of compds. 4b and 4c resulted in formation of two alkenes by 1,2-H shifts and formation of azines by reactions of the carbenes with their precursors. The low selectivity of 4b was rationalized in terms of structural data from single-crystal X-ray diffraction anal., which revealed two disordered diazirine conformers and close Cl···N contacts between adjacent mols. Rapid conformational equilibration in the solid state was also suggested by solid-state 13C CPMAS NMR. Similar structural effects are also postulated to account for the solid-state reactivity of 4c.

IT 524068-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(PTC oxidation; the influence of conformational disorder and intermol Cl···N:N interactions on the solid-state reactivity of singlet chlorocarbenes formed in photolysis of 3-chlorodiazirines)

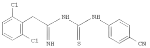
L4 ANSWER 13 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 524068-77-7 CAPLUS
CN [1,1'-Biphenyl]-4-ethanimidamide, α,α-dimethyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

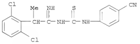
L4 ANSWER 14 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:628975 CAPLUS
DOCUMENT NUMBER: 135:371498
TITLE: Evolution of anti-HIV drug candidates. Part 1: From α-Anilinophenylacetamide (α-APA) to imidoyl thiourea (ITU)
AUTHOR(S): Ludovici, D. W.; Kukla, M. J.; Grous, P. G.; Krishnan, S.; Andries, K.; de Bethune, M.-P.; Azijn, H.; Pauwels, R.; De Clercq, E.; Arnold, E.; Janssen, P. A. J.
CORPORATE SOURCE: Janssen Research Foundation, Spring House, PA, 19477, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(17), 2225-2228
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:371498
GI



I

AB Stemming from work on a previous clin. candidate, loviride, and other α-APA derivs., a new series of potent non-nucleoside reverse transcriptase inhibitors (NNRTIs) has been synthesized. The ITU analogs, which contain a unique diarylated imidoyl thiourea, e.g. (I), are very active in inhibiting both wild-type and clin. important mutant strains of HIV-1.
IT 374063-57-7P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and activity of imidoyl thioureas as non-nucleoside reverse transcriptase inhibitors)
RN 374063-57-7 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-N-[[(4-cyanophenyl)amino]thioxomethyl]-α-methyl- (CA INDEX NAME)

L4 ANSWER 14 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:265374 CAPLUS
DOCUMENT NUMBER: 134:280609
TITLE: Preparation of N-[α-(cyclopropylmethoximino)aralkyl]phenylacetamides and analogs as agrochemical fungicides
INVENTOR(S): Rheinheimer, Joachim; Eicken, Karl; Rose, Ingo; Grote, Thomas; Ammermann, Eberhard; Speakman, John-Bryan; Strathmann, Siegfried; Lorenz, Gisela
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001025187	A2	20010412	WO 2000-EP9744	20001005
WO 2001025187	A3	20011101		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2386513	A1	20010412	CA 2000-2386513	20001005
EP 1218339	A2	20020703	EP 2000-992195	20001005
EP 1218339	B1	20031001		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003516933	T	20030520	JP 2001-528135	20001005
AT 251123	T	20031015	AT 2000-992195	20001005
ES 2210032	T3	20040701	ES 2000-992195	20001005
TW 229662	B	20050321	TW 2000-89120773	20001005
US 6881742	B1	20050419	US 2002-89148	20020327
US 20050187265	A1	20050825	US 2005-61470	20050222
US 7101900	B2	20060905		

PRIORITY APPLN. INFO.:
DE 1999-19948266 A 19991006
WO 2000-EP9744 W 20001005
US 2002-89148 A3 20020327

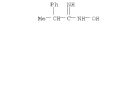
OTHER SOURCE(S): MARPAT 134:280609
AB R1ZC(:NOR)NHCOR2 (R = cyclopropylmethyl)[I; R1 = (un)substituted Ph, -pyridyl, -thienyl; R2 = (un)substituted phenyl-, -thienyl-, -pyrazolylalkyl; Z = (un)substituted (heteroatom- or cyclopropylene-interrupted) alkylene] were prepared. Thus, HONH2 was added to 2,6-Cl2C6H3CH2CN and the resulting amidoxime O-alkylated by cyclopropylmethyl bromide to give, after N-acylation, I (R1 = 2,6-Cl2C6H3, R2 = CH2Ph, Z = CH2). Data for biol. activity of I were given.
IT 333748-79-1P

L4 ANSWER 15 OF 6CP CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-[4-(cyclopropylmethoxyimino)-alkyl]phenylacetamides and analogs as agrochem. fungicides)

RN 333748-79-1 CAPLUS
CN Benzeneacetamide, N-[1-[(cyclopropylmethoxy)amino]-2-phenylpropylidene]- (9CI) (CA INDEX NAME)

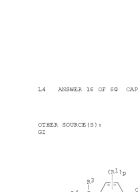
IT 42191-51-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-[w-[cyclopropylmethoxalimo]aralkyl]phenylacetamides and analogs as agrochem. fungicides)

RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-a-methyl- (CA INDEX NAME)



L4 ANSWER 16 OF 6CP CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
EP 1999-126235 A 19991227
WO 2000-EP7358 W 20000731

OTHER SOURCE(S): MARPAT 134:178571
GI



AB The title compds. (I) [p = 0-4; X = O, NR5, or a direct bond; or XR2 taken together = CH; R1 = independently C(O)ER14, (un)substituted alkyl, halo, OR, SR, alkoxy, alkylthio, alkylsulfonyl, aryl, CN, NO2, heterocyclyl, R4, or NR7R8; R2 = heterocyclyl, (un)substituted cycloalkyl, alkoxy, or alkylthio, heterocyclyloxy, heterocyclylthio, etc.; R3 and R4 = independently H or (cyclo)alkyl; or R3 and R4 taken together form an alkenediyl; R5 = H or alkyl; R6 = (un)substituted (cyclo)alkylsulfonyl, amino(alkyl)sulfonyl, heterocyclylsulfonyl, etc.; R7 and R8 = independently H, (cyclo)alkyl, (di)hydroxyalkyl, mercaptoalkyl, aryl(alkyl), alkyl(oxy)alkyl, alkylthio)carbonyl, aryl(thio)carbonyl, heterocyclo(thio)carbonyl, C(O)ER14, or (un)substituted aminocarbonyl, etc.; or R7 and R8 together with the N to which they are attached form a pyrrolizone, piperidinone, or hexahydrotriazinone; R14 = H, alkynyl, or (un)substituted (alkyl)aryl, alkyl, alkenyl, heterocyclyl, etc.; E = O, S, NR, CR2O, or CR2S; or ER14 taken together = CH2CN or CH2PO(OR)2 and its esters] and their N-oxides, pharmaceutically acceptable salts, or stereochem. isomers were prepared as selective chemokine inhibitors. For example, 2,6-dichloro-4-(4,5-dihydro-3,5-dioxo-1,2,4-triazin-2(3H)-yl)-a,a-dimethylbenzeneethanethioamide was coupled with N1 β-bromo-γ-oxobenzenebutanoic (65.5%), cyclized to form the thiazolecarbic acid (77%), and esterified with 3-bromodihydro-2(3H)-furanone to give II. As selective interleukin 5 (IL-5) and monocyte

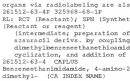
L4 ANSWER 16 OF 6CP CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:115140 CAPLUS
DOCUMENT NUMBER: 134:178571
TITLE: Preparation of 8-azaaralkyl derivatives as interleukin-5 inhibitors
INVENTOR(S): Lorrange, Jean Fernand Armand; Freyne, Eddy Jean Edgard; Berneen, Frederik Dirk; Portin, Jerome Michel Claude; Coessemans, Erwin
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 143 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001013944	A1	20010215	WO 2000-EP7358	20000731
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2380759	A1	20010215	CA 2000-2380759	20000731
BR 2000013014	A	20020416	BR 2000-13014	20000731
EP 1204471	A1	20020522	EP 2000-946015	20000731
EP 1204471	B1	20060301		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200310	T2	20020621	TR 2002-310	20000731
HU 2002002692	A2	20021228	HU 2002-2692	20000731
HU 2002002692	A3	20030328		
JP 2003506451	T	20030218	JP 2001-515675	20000731
ES 2260057	A	20060401	ES 2000-946015	20000731
NZ 516506	A	20040227	NZ 2000-516506	20000731
AU 7950047	B2	20050224	AU 2000-61609	20000731
AT 319811	T	20060315	AT 2000-946015	20000731
ES 2260031	T3	20061101	ES 2000-946015	20000731
TW 271404	B	20070121	TW 2000-89115824	20000804
KR 795404	B1	20080116	KR 2002-709704	20020117
BG 106367	A	20020930	BG 2002-106367	20020130
IN 2002MN00144	A	20050210	IN 2002-MN144	20020131
NO 2002000565	A	20020326	NO 2002-565	20020205
NO 322396	B1	20060925		
ZA 2002001007	A	20030501	ZA 2002-1007	20020205
MX 2002PA01343	A	20020722	MX 2002-PA1343	20020206
US 2003114453	A1	20030619	US 2002-75876	20020214
US 6911444	B2	20050628		
HK 1048634	A1	20050930	HK 2003-100718	20030128
PRIORITY APPLN. INFO.:			EP 1999-870170	A 19990806

L4 ANSWER 16 OF 6CP CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
chemotactic protein-1 and -3 (MCP-1 and MCP-3) inhibitors, I are useful for treating eosinophil-dependent inflammatory diseases, esp. bronchial asthma (no data). Processes using I for marking receptors and imaging organs via radiolabeling are also claimed.

IT 261512-63-4P 325968-68-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of IL-5 inhibiting thiazolylalkylphenyl-6-azauracil deriv. by coupling of 4-diazotisinyl-a,a-dimethylbenzenesthanthioamides with w-omalkyl halides, cyclization, and addition of functionally substituted groups)

RN 261512-63-4 CAPLUS
CN Benzeneethanimidamide, 4-amino-2,6-dichloro-N-hydroxy-a,a-dimethyl- (CA INDEX NAME)



RN 325968-68-1 CAPLUS
CN Benzamide, N-[2-[4-amino-2,6-dichlorophenyl]-1-imino-2-methylpropyl]-2-methyl- (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 17 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

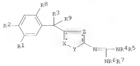
ACCESSION NUMBER: 2001:63983 CAPLUS
DOCUMENT NUMBER: 134:131527
TITLE: Preparation and effect of heteroaromatic ring compounds against autoimmune disorders and chronic inflammation
INVENTOR(S): Nakatsuka, Masashi; Nakatani, Shogo; Okada, Shin-ichiro; Tsuboi, Katsunori; Nishikaku, Fumio
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 190 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001005774	A1	20010125	WO 2000-JP4616	20000710
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2377527	A1	20010125	CA 2000-2377527	20000710
EP 1201661	A1	20020502	EP 2000-944389	20000710
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.:
JP 1999-201447 A 19990715
JP 2000-58217 A 20000303
WO 2000-JP4616 W 20000710

OTHER SOURCE(S): MARPAT 134:131527
GI

L4 ANSWER 17 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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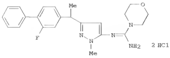
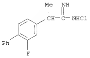


II

AB Title compds. [I; R1 = F, C6H5CO, C6H5CHO2(CH2)2; R2 = H, C6H5; R3 = H, CH3; R4 = H, CH3; R5 = CH3, CH2CH2N[(CH2)2]O; R6 = H, CH3; R4-R5 = CH2CH2OCH2CH2, CH2CH2SCH2CH2, CH2CH2S(:O)(:O)CH2CH2; R6 = H, CH3; R7 = CH3, H, CH2CH2OH, CN, C(NH)N[(CH2)2]2O; R5-R7 = CH2CH2, CH2CH2CH2, CH2CHOHCH2; R6-R7 = CH2CH2OCH2CH2; R8 = H, CH3; R9 = H, CH3; X = N, NCH3, S; Y = NCH3, S, NH, NSO2C6H5; Z = CH, O, S, N; dotted line = single, double bond] and pharmaceutically acceptable salts exhibiting excellent phys. properties and potent ameliorative effects against both immune disorders and chronic inflammation are prepared Thus, the title compound II was prepared and tested.
IT 321879-91-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and effect of heteroarom. ring compds. against immune disorders and chronic inflammation)
RN 321879-91-8 CAPLUS
CN [1,1'-Biphenyl]-4-ethanimidamide, N-chloro-2-fluoro-α-methyl- (CA INDEX NAME)

L4 ANSWER 17 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:900841 CAPLUS
DOCUMENT NUMBER: 134:37031
TITLE: FVIIA/TF activity inhibiting compounds
INVENTOR(S): Jakobsen, Palle; Persson, Egon
PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000077246	A2	20001221	WO 2000-DK316	20000613
WO 2000077246	A3	20010222		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1192270	A2	20020403	EP 2000-934951	20000613
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003530819	T	20031021	JP 2001-503687	20000613
US 6238878	B1	20010529	US 2000-616010	20000713
US 6444434	B1	20020903	US 2001-844828	20010427
US 20030073695	A1	20030417	US 2002-262826	20021002

PRIORITY APPLN. INFO.:
DK 1999-840 A 19990614
US 1999-139714P P 19990617
DK 1999-910 A 19990625
US 1999-141416P P 19990629
DK 1999-1241 A 19990903
US 1999-152863P P 19990908
US 2000-577731 B1 20000523
WO 2000-DK316 W 20000613
US 2000-616010 A1 20000713

AB The invention relates to compds. inhibiting the activation of FX to FXa by TF/FVIIa. The compds. are anticoagulants. The invention also relates to a method of identifying a drug candidate.
IT 313236-51-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

L4 ANSWER 19 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(Uses)
(PYCIA/TF activity inhibiting compds.)
RN 313236-51-6 CAPLUS
CN Benzenecarbohximidamide, 4-methyl-4-[2-methyl2propyl)-N-[2-[4-[2-methylpropyl]phenyl]propyl]- (CA INDEX NAME)

L4 ANSWER 19 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 19 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	2000:841977 CAPLUS
DOCUMENT NUMBER:	134:25351
TITLE:	Heterocyclic phospholipase A2-specific inhibitors, their preparation, their use in treatment of inflammation, and pharmaceutical and cosmetic compositions containing them
INVENTOR(S):	Asseqha, Leon; Beynens, Francoise; Dong, Chang-Chi; Godfroid, Jean-Jacques
PATENT ASSIGNEE(S):	Universite Paris 7 - Denis Diderot, Fr.
SOURCE:	PCT Int. Appl., 64 pp. CODEN: PIXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	French
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000071118	A1	20001130	WO 2000-FR1306	20000519
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DO, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2793791	A1	20001124	FR 1999-6366	19990519
FR 2793791	B1	20020125		
PRIORITY APPLN. INFO.:			FR 1999-6366 A	19990519

OTHER SOURCE(S): MARPAT 134:25351

AB The invention provides phospholipase A2 inhibitor heterocyclic compds. (Markush included). The compds. are capable of acting on PLA2 and are advantageously secreted nonpancreatic PLA2-specific inhibiting compds. completely inactive towards pancreatic PLA2. The invention also provides a method for preparing the compds., pharmaceutical and cosmetic compns. containing them, and their use in particular for treating inflamatory pathologies.

IT 310869-86-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction; heterocyclic phospholipase A2-specific inhibitor

preparation, use in treatment of inflammation, and pharmaceutical and cosmetic compns. containing them)

RN 310869-86-4 CAPLUS

CN Benzenesthaninimidamide, N-hydroxy-4-methyl-4-(tetradecyloxy)- (CA INDEX NAME)

L4 ANSWER 20 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

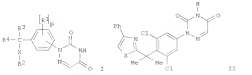
ACCESSION NUMBER:	2000:190770 CAPLUS
DOCUMENT NUMBER:	132:222555
TITLE:	Preparation of interleukin-5 inhibiting 6-azauracil derivatives
INVENTOR(S):	Freyne, Eddy Jean Edgard; Lacrampe, Jean Fernand Armand; Deroose, Frederik Dirk; Venet, Marc Gaston
PATENT ASSIGNEE(S):	Janssen Pharmaceutica N.V., Belg.
SOURCE:	Eur. Pat. Appl., 37 pp. CODEN: EPXLDW
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 997265	A1	20000322	EP 1998-203148	19980918
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2343390	A1	20000330	CA 1999-2343390	19990914
WO 2000017195	A1	20000330	WO 1999-EP6776	19990914
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9960825	A1	20000410	AU 1999-60825	19990914
AU 769133	B2	20040115		
EP 1114046	A1	20010711	EP 1999-947336	19990914
EP 1114046	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002526495	T	20020820	JP 2000-574184	19990914
AT 238301	T	20030515	AT 1999-947336	19990914
ES 2195859	T3	20040201	ES 1999-947336	19990914
US 2001020177	A1	20010214	US 2001-812731	20010319
US 6894046	B2	20050517		
PRIORITY APPLN. INFO.:			EP 1998-203148 A	19980918
			WO 1999-EP6776 W	19990914

OTHER SOURCE(S): MARPAT 132:222555

GI

L4 ANSWER 20 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



AB The title compds. [I; p = 0-4; X = O, S, NR5, a direct bond; Y = O, S, NR5, NOR; R1 = alkyl, halo, polyhaloalkyl, etc.; R2 = Het1, cycloalkyl, alkyl, and if X = O, S, NR5, then R2 may also represent aminocarbonyl, aminothioxocarbonyl, alkylcarbonyl, etc.; R3, R4 = H, alkyl, cycloalkyl; R3R4 = alkanediyl; R5 = H, alkyl; Het1 = (un)substituted heterocycle], useful for treating eosinophil-dependent inflammatory diseases, and having a receptor, were prepared and formulated. E.g., a multi-step synthesis of 2,3,4-triazine-5,7(2H,6H)-dione II which showed 90.1% inhibition of IL-5 production, was given.

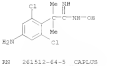
IT 261512-47-4P 261512-64-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of interleukin-5 inhibiting 6-azauracil derivs.)

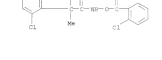
RN 261512-64-5 CAPLUS

CN Benzeneethanimidamide, 4-amino-2,6-dichloro-N-hydroxy-a,a-dimethyl- (CA INDEX NAME)



RN 261512-64-5 CAPLUS

CN Benzeneethanimidamide, 4-amino-2,6-dichloro-N-[(2-chlorobenzoyl)oxy]-a,a-dimethyl- (9CI) (CA INDEX NAME)



L4 ANSWER 21 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:746378 CAPLUS

DOCUMENT NUMBER: 132:293711

TITLE: Synthesis of oxazolo[4,5-c]-5,7,4-triazol-5-ones

AUTHOR(S): Geffken, Detlef; Bols:, Carsten; Willrodt, Jake

CORPORATE SOURCE: Institute of Pharmacy, Department of Pharmaceutical Chemistry, University of Hamburg, Hamburg, 20146, Germany

SOURCE: Heterocyclic Communications (2000), 6(1), 21-24

CODEN: HCOMDL; ISSN: 0793-0283

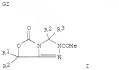
PUBLISHER: Freund Publishing House Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:293711

GI



AB Treatment of 4-hydrazono-2-oxazolidinones with acetic anhydride afforded novel 2-acetylmelazole[4,5-e]-1,2,4-triazol-5-ones (I; R1 = Me, R2 = Me, Ph, R, 4-fluorophenyl; CR2R3 = CHPh, cyclopentylidene, CMe2, CPh2, tetrahydropyran-4-ylidene, tetrahydrothiopyran-4-ylidene) in good yields.

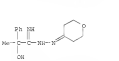
IT 264124-02-2P 264124-09-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclic carbweglation of)

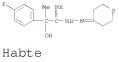
RN 264124-09-9 CAPLUS

CN Benzeneethanimidic acid, a-hydroxy-a-methyl-, (tetrahydro-4H-pyran-4-ylidene)hydrazide (9CI) (CA INDEX NAME)



RN 264224-09-6 CAPLUS

CN Benzeneethanimidic acid, 4-fluoro-a-hydroxy-a-methyl-, (tetrahydro-4H-thiopyran-4-ylidene)hydrazide (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

IT 160154-90-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with tetrahydropyranone)

RN 160154-90-5 CAPLUS

CN Benzeneethanimidic acid, a-hydroxy-a-methyl-, hydrazide (CA INDEX NAME)

IT 264124-07-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with tetrahydrothiopyranone)

RN 264124-07-4 CAPLUS

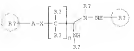
CN Benzeneethanimidic acid, 4-fluoro-a-hydroxy-a-methyl-, hydrazide (CA INDEX NAME)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:27808 CAPLUS
DOCUMENT NUMBER: 130:81527
TITLE: Preparation of novel amidrazone derivatives having antifungal activity
INVENTOR(S): Kageyama, Shunji; Kontani, Toru; Fujii, Masahiro; Igarashi, Kiyoshi; Yamamoto, Osamu
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9858905	A1	19981230	WO 1998-JP2817	19980624
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, GW, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9879330	A	19990104	AU 1998-79330	19980624
PRIORITY APPLN. INFO.:			JP 1997-168354 A	19970625
			WO 1998-JP2817 W	19980624

OTHER SOURCE(S): MARPAT 130:81527
GI



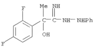
I

AB Amidrazone derivs. of formula [I; wherein the ring Ra represents: (1) an optionally substituted monocyclic to tricyclic aromatic hydrocarbon, (2) an optionally substituted monocyclic to tricyclic saturated or unsatd. hetero ring containing one or more hetero atoms selected from N, O and S, (3) an optionally substituted and optionally cross-linked cycloalkyl, or (4) an optionally substituted and optionally cross-linked cycloalkenyl; the ring Rb represents (1) an optionally substituted monocyclic to tricyclic aromatic hydrocarbon or (2) an optionally substituted monocyclic to tricyclic saturated

L4 ANSWER 22 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
or unsatd. hetero ring contg. one or more hetero atoms selected from N, O and S; one of Rc and Rd represents H and the other is not present; Re represents H or OH; Rf represents H or lower alkyl, or YRa1; the dotted line "...." represents a single bond or a double bond; n is 1 to 8; A represents a bond or a lower alkylene optionally substituted by a lower alkyl; and X represents a bond, CO, CO2, CONRg, COCONRg1, CH:CHCONRg2, NRg3, NRg4CO, NRg5CO2, NRg6CONRg7, O, O2C, O2CNRg8, OCH2CONRg9, S, SO, SO2, SO2NRg10, or SO2NRg11CO; wherein Rg and Rg1 - Rg11 represent H, lower alkyl, or YRa2; Ra1 and Ra2 represents the same group as Ra; Y represents a single bond, CH2, or CO; a proviso given] or pharmaceutically acceptable salts thereof are prepd. Also claimed are pharmaceutical compns. thereof and a method for prevention or treatment of fungal or deep fungal infection by administration of I. These compds. I are useful for the treatment or prevention of fungal infection, in particular, deep fungal infection attributable to fungi, such as Candida, Aspergillus, and Cryptococcus. Thus, 2-(2-chloro-5-fluoro-6-oxo-1,6-dihydropyrimidin-1-yl)acetonitrile was treated with EtOH and HCl(g) in CHCl3 at 5° for 2 days to give a crude imidate which was condensed with 4-chlorophenylhydrazine hydrochloride in EtOH in the presence of EtONa at room temp. overnight to give the title compd., 2-pyrimidinyl-N-phenylacetamidrazone (II). II showed 80% min. inhibitory concn. of 0.31, 0.31, and 0.63 μg/mL against Candida albicans TIMM1768, Cryptococcus neoformans TIMM0362, and Aspergillus fumigatus TIMM1776, resp.
IT 218918-69-5P 218918-70-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel amidrazone derivs. having antifungal activity)
RN 218918-69-5 CAPLUS
CN Benzeneethanimidic acid, 2,4-difluoro-α-hydroxy-α-methyl-, 2-phenylhydrazide, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 218918-68-4
CMF C15 H15 F2 N3 O

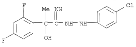


CM 2

CRN 144-62-7
CMF C2 H2 O4

L4 ANSWER 22 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

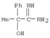
RN 218918-70-8 CAPLUS
CN Benzeneethanimidic acid, 2,4-difluoro-α-hydroxy-α-methyl-, 2-(4-chlorophenyl)hydrazide, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

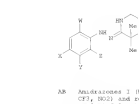
L4 ANSWER 23 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:573216 CAPLUS
DOCUMENT NUMBER: 129:196039
TITLE: Racemic 2-Hydroxy-2-phenylpropanamidinium chloride and (S)-2-Hydroxy-2-phenylbutanamidinium (R)-2-Hydroxy-2-phenylethanoate
AUTHOR(S): Barnes, John C.; Weakley, Timothy J. R.
CORPORATE SOURCE: Dep. Chem., Univ. Dundee, Dundee, DD1 4HN, UK
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1998), C54(8), 1170-1173
CODEN: ACSCEE; ISSN: 0108-2701
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In 2-hydroxy-2-phenylpropanamidinium chloride, C9H13-N2O+.Cl-, the anion plays a central role in the H-bond network, chelating to one amidinium group and forming intermol. links to neighboring NH2 and OH- groups. The central feature in (S)-2-hydroxy-2-phenylbutanamidinium (R)-2-hydroxy-2-phenylethanoate, C10H15N2O+.C8H7O3-, is a ring linking the cation and anion through two H bonds. The structure is extended by intra- and inter-mol. H bonds. Crystallog. data are given.
IT 92442-87-0
RL: PRP (Properties)
(crystal structure of)
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



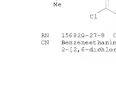
● HCl

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:294826 CAPLUS
DOCUMENT NUMBER: 128:13472
TITLE: Anthranamides: a new class of coleopteran insecticides
AUTHOR(S): Furch, J. A.; Kuhn, D. G.; Hunt, David A.; Asselin, M.; Baffic, S. F.; Diehl, R. E.; Palmer, T. L.; Trotter, S. E.
CORPORATE SOURCE: Cyanamid Agric. Res. Cent., Am. Cyanamid Corp., Princeton, NJ, 08540-0400, USA
SOURCE: ACS Symposium Series (1998), 684(Synthesis and Chemistry of Agrochemicals V), 178-194
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Anthranamides I (W = S, Cl, Br; X = H, CF3; Y = H, NO2, CF3; Z = H, Cl, Br, CF3, NO2) and related compds. were developed as insecticides specific against Coleoptera, especially Diabrotica undecimpunctata, with low toxicity to Lepidoptera, Acarina, fish, birds and mice. The synthesis of the compds. is outlined.
IT 156820-05-2 156820-27-8
RL: AOR (Agricultural use); BIOL (Biological study); USES (Uses) (insecticide specific against Coleoptera)
RN 156820-05-2 CAPLUS
CN Benzeneethanimidic acid, N-ethyl-a,a-dimethyl-, 2-(2,6-dichloro-4-(trifluoromethyl)phenyl)hydrazide (CA INDEX NAME)



RN 156820-27-8 CAPLUS
CN Benzeneethanimidic acid, 4-chloro-N-ethyl-a,a-dimethyl-, 2-(2,6-dichloro-4-(trifluoromethyl)phenyl)hydrazide (CA INDEX NAME)

L4 ANSWER 25 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:172229 CAPLUS
DOCUMENT NUMBER: 128:192667
TITLE: Preparation of substituted aromatic compounds as inhibitors of tumor necrosis factor and cyclic AMP phosphodiesterase
INVENTOR(S): Be, Wei; Bolme, Christopher; Huang, Fu-Chih; Dyer, Steven W.; Moriarty, Kevin; Labaudiniere, Richard
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer Pharmaceuticals Inc., USA; Be, Wei; Bolme, Christopher; Huang, Fu-Chih; Dyer, Steven W.; Moriarty, Kevin; Labaudiniere, Richard
SOURCE: PCT Int. Appl., 154 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

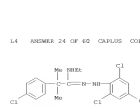
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9805327	A1	19980212	WO 1997-US13343	19970722
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN
RN: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
AU 9739899	A	19980225	AU 1997-38990	19970722
PRIORITY APPLN. INFO.:			US 1996-23169	P 19960805
			WO 1997-US13343	W 19970722

OTHER SOURCE(S): MARPAT 128:192667
GI

* STRUCTURAL DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB This invention is directed to compds. of formula [I; ring A = Q10, Q11; Ar1 = Q12, Q13, Q14; ring Ar2 = (un)substituted fused Ph or fused monocyclic heteroaryl; R = (un)substituted alkyl, acyl, heteroaralkyl, arylsulfonyl, heteroarylsulfonyl, etc.; R1 = carboxyalkyl, alkoxycarbonylalkyl, N-(un)substituted carbamoylalkyl, cyanoalkyl, (un)substituted aralkyl or heteroaralkyl; R2 = (un)substituted lower alkyl; R3 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, or oxoalkyl, (un)substituted or optionally oxidized cyclothioalkyl or cyclothioalkenyl; R4, R6 = H, (un)substituted lower alkyl; R5 = (un)substituted alkyl, alkoxy, cycloalkyl, or heterocyclyl, alkoxycarbonyl, cyano, (un)substituted carbamoyl, (un)substituted aryl or heteroaryl, or CO2R where n is other than 0; R7 = H, alkoxy, (un)substituted cycloalkyl, cycloalkenyl, cycloalkoxy, cycloalkenyloxy, aryl, heteroaryl, aryloxy, heteroaryloxy, aralkyloxy, heteroaralkyloxy, alkylthio, or alkylsulfonyl, etc.; Q7, Q8 = CH2, O-(un)substituted CHOR, CO; Q7, Q4, Q5, Q8 = H, optionally halo-substituted CH; Q6 = N, CH; Q7-C-Q8 = N-(un)saturated NHCH-N, O-CH-CH, CH-CH-O, O-CH2CH2, CH2CH2O, S-CH2-

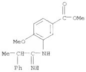
L4 ANSWER 24 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
= H or S'2'' = O or N, Z1, Z2 = direct bond, O, N, S; Z3 = NO2, direct bond; Z4 = direct bond, O, S, NH; Z5 = direct bond, (un)substituted lower alkenyl; n, n = 0, 1; p = 1-3; q = 0-5] or hydrate, solvate, N-oxide, or prodrug thereof or a pharmaceutically acceptable salt thereof are. They are esp. useful for inhibiting the prodn. or physiol. effects of tumor necrosis factor (TNF) and inhibit cAMP phosphodiesterase and are useful for the treatment of disease states assocd. with abnormally high physiol. levels of cytokines such as TNF or those assocd. with pathol. (e.g. asthma as bronchodilators or inflammation) conditions that are modulated by inhibiting enzymes such as cAMP phosphodiesterase (no data). In particular, they are used for treating a disease state capable of being modulated by inhibiting TNF, e.g., joint inflammation, arthritis, rheumatoid arthritis, rheumatoid spondylitis and osteoarthritis, sepsis, septic shock, gram neg. sepsis, toxic shock syndrome, acute respiratory distress syndrome, asthma, bone resorption diseases, reperfusion injury, graft vs. host reaction, allograft rejection malaria, myalgias, HIV, AIDS, cachexia, Crohn's disease, ulcerative colitis, pyresis, systemic lupus erythematosus, multiple sclerosis, type I diabetes mellitus, psoriasis, Behcet's disease, anaphylactoid purpura nephritis, chronic glomerulonephritis, inflammatory bowel disease, and leukemia. They are also used for treating a pathol. condition assocd. with a function of cAMP phosphodiesterase, eosinophil accumulation or function of the eosinophil, e.g., asthma, atopic dermatitis, urticaria, allergic rhinitis, psoriasis, rheumatic arthritis, ulcerative colitis, Crohn's disease, adult respiratory distress syndrome, diabetes insipidus, keratosis, dermatitis, cerebral senility, multiinfarct dementia, senile dementia, memory impairment assocd. with Parkinson's disease, cardiac arrest, stroke, and intermittent claudication. The present invention is also directed to their pharmaceutical use, pharmaceutical compns. contg. the compds., and methods of their prepn. Thus, 2-[3-cyclopentyloxy-4-methoxyphenyl]-5-hydroxymethyl-2'-[4-pyridylmethyl]indan-1,3-dione was treated with NaH in THF, tosylated by tosyl chloride at 0° to room temp. for 2 h, and then condensed with 1-methylpiperazine in the K2CO3 in acetone at room temp. for 4 days the presence of K2CO3 in acetone to give the title compd., piperazinylmethylpyridylmethylindanedione deriv. (I).
IT 202189-52-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted aromatic compds. as inhibitors of tumor necrosis factor and cAMP phosphodiesterase)
RN 202189-52-7 CAPLUS
CN Benzoic acid, 3-[[3-amino-2-phenylpropyl]amino]-4-methyl ester (CA INDEX NAME)

L4 ANSWER 25 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:31305 CAPLUS
DOCUMENT NUMBER: 128:102087
TITLE: Substituted azabicyclic compounds and their use as inhibitors of the production of TNF and cyclic AMP phosphodiesterase
INVENTOR(S): Cox, Paul Joseph; Bower, Shelley; Aldous, David John; Astles, Peter Charles; McGarry, Daniel Gerard; Hulme, Christopher; et al.
PATENT ASSIGNEE(S): Regan, John Robinson, UK; Huang, Fu-Chih; Rhone-Poulenc Rorer Ltd.; Cox, Paul Joseph; Bower, Shelley; et al.
SOURCE: PCT Int. Appl., 355 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

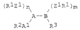
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9748697	A1	19971224	WO 1997-GB1639	19970619
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2258728	A1	19971224	CA 1997-2258728	19970619
AU 9731026	A	19980107	AU 1997-31026	19970619
ZA 9705446	A	19981221	ZA 1997-5446	19970619
EP 934307	A1	19990811	EP 1997-926148	19970619
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 2000509719	T	20000802	JP 1998-502503	19970619
US 6303600	B1	20011016	US 1998-216392	19981218
US 6800645	B1	20041005	US 2000-612530	20000707
US 20020173527	A1	20021121	US 2002-109629	20020328
US 20050038069	A1	20050217	US 2004-933077	20040901
US 7329675	B2	20080212		

PRIORITY APPLN. INFO.:

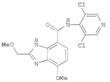
GB 1996-12760	A	19960619
US 1996-23047P	P	19960802
WO 1997-GB1639	W	19970619
US 1998-216392	A1	19981218
US 2000-612530	A3	20000707

OTHER SOURCE(S): MARPAT 128:102087
GI

L4 ANSWER 26 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



I



II

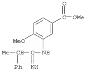
AB The invention is directed to physiol. active compds. of formula I [wherein AB = fused bicyclic ring system, of approx. 10-13 ring members, wherein A = azaheterocycle ring and B = azaheteroaryl or optionally halo-substituted benzene ring; R1 = H, (hydroxy- or halo-substituted) alkyl, and also alkenyl, alkynyl, or CHO when Z1 = bond; R2 = H, alkenyl, alkoxy, alkyl, aryl, aryloxy, cyano, etc.; R3 = wide variety of sidechains and functional groups; A1 = bond, (un)substituted alkylene, alkenylene, alkynylene; Z1 = bond, O, S, NH; m, n = 0, 1; provided that (n+m) = 1] and their N-oxides, prodrugs, and pharmaceutically acceptable salts and solvates. I inhibit the production or physiol. effects of TNF, and inhibit cAMP phosphodiesterase (PDE IV). The invention is also directed to pharmaceutical compns. comprising I, their pharmaceutical use, and methods for their preparation For instance, 7-methoxy-2-(methoxymethyl)-3H-benzimidazole-4-carboxylic acid (preparation given) was treated with O-benzotriazol-1-yl-N,N,N',N'-bis(tetramethylene)uronium tetrafluoroborate to give the 1-benzotriazolyl ester, which was amidated with 4-amino-3,5-dichloropyridine in THF (after treatment of the latter with Na diethylaluminate) to give the title compound II. Compds. I had IC50 of 10-5 to 10-10 M against guinea pig macrophage PDE IV, with 50- to 10,000-fold selectivity for PDE IV vs. PDE I, II, III, or V. The compds. also inhibited antigen-induced bronchoconstriction in rats by up to 89% at oral doses of 10 mg/kg.

IT 201287-52-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azabicyclic compds. as inhibitors of TNF production and PDE IV)

RN 201287-52-7 CAPLUS

CN Benzoic acid, 3-[(1-imino-2-phenylpropyl)amino]-4-methoxy-, methyl ester (CA INDEX NAME)

L4 ANSWER 26 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

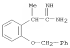


L4 ANSWER 27 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:464318 CAPLUS
DOCUMENT NUMBER: 125:114673
ORIGINAL REFERENCE NO.: 125:21527a,21530a
TITLE: Preparation of benzyloxyphenylalkylbenzoates and related compounds as analgesics and prostaglandin antagonists
INVENTOR(S): Breault, Gloria Ann; Oldfield, John; Tucker, Howard; Warner, Peter
PATENT ASSIGNEE(S): Zeneca Limited, UK
SOURCE: PCT Int. Appl., 172 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

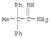
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9611902	A1	19960425	WO 1995-GB2417		19951012
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ					
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
ZA 9508622	A	19960412	ZA 1995-8622		19951012
AU 9536162	A	19960506	AU 1995-36162		19951012
EP 733033	A1	19960925	EP 1995-933542		19951012
EP 733033	B1	19991222			
R: CH, DE, FR, GB, IT, LI					
JP 09511529	T	19971118	JP 1995-513027		19951012
US 5811459	A	19980922	US 1996-647977		19960604
PRIORITY APPLN. INFO.:			GB 1994-20557	A	19941012
			WO 1995-GB2417	W	19951012

OTHER SOURCE(S): MARPAT 125:114673
AB Ortho-substituted Ph, naphthyl, and heterocyclic ethers (> 600 compds.) were prepared for use in treating pain mediated by the E-type prostaglandins (no data). Thus, 2-PhCH2OC6H4(CH2)3C6H4CO2H-4 was prepared from 2-HOC6H4Ac and 4-OCHC6H4CO2Me in 5 steps.
IT 179256-35-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzyloxyphenylalkylbenzoates and related compds. as analgesics and prostaglandin antagonists)
RN 179256-35-0 CAPLUS
CN Benzeneethanimidamide, α-methyl-2-(phenylmethoxy)- (CA INDEX NAME)

L4 ANSWER 27 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



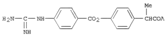
L4 ANSWER 28 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:968831 CAPLUS
DOCUMENT NUMBER: 124:175546
ORIGINAL REFERENCE NO.: 124:32547a,32550a
TITLE: Conversion of 'obstinate' nitriles to amidines by Garigipati's reaction
AUTHOR(S): Moss, Robert A.; Ma, Wei; Merrer, Dina C.; Xue, Song
CORPORATE SOURCE: Dep. Chem., Rutgers, The State Univ. New Jersey, New Brunswick, NJ, 08903, USA
SOURCE: Tetrahedron Letters (1995), 36(48), 8761-4
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:175546
AB Reaction with methylchloroaluminum amide readily converts sterically hindered nitriles, e.g., 1-adamantanecarbonitrile, to amidines.
IT 173601-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amidines by Garigipati amination of sterically hindered nitriles)
RN 173601-37-1 CAPLUS
CN Benzeneethanimidamide, α-methyl-α-phenyl- (CA INDEX NAME)



L4 ANSWER 29 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:638226 CAPLUS
DOCUMENT NUMBER: 123:55494
ORIGINAL REFERENCE NO.: 123:9982h,9983a
TITLE: Preparation of propionic acid derivatives as serine protease inhibitors
INVENTOR(S): Muramatsu, Mutsumi; Tamura, Toshiaki; Yanagi, Toshiharu
PATENT ASSIGNEE(S): Teikoku Chemical Industries Co. Ltd., Japan
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9413631	A1	19940623	WO 1993-JP1783		19931209
W: JP, KR, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
EP 673924	A1	19950927	EP 1994-902092		19931209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
PRIORITY APPLN. INFO.:			JP 1992-360711	A	19921210
			JP 1993-318909	A	19931112
			WO 1993-JP1783	W	19931209

OTHER SOURCE(S): MARPAT 123:55494
GI



I

AB 2-[P-(p-guanidinobenzoyloxy)phenyl]propionic acid derivs. represented by general formula [I; A = OH, C1-6 lower alkoxy, NR1R2, C1-8 lower alkoxy which may be substituted by halogen, optionally substituted aryl, COB or succinimido; R1, R2 = H, C1-8 lower alkyl, optionally substituted aralkyl or alternatively R1 and R2 are combined together with the adjacent nitrogen atoms to represent a heterocycle; B = OH, C1-8 lower alkyl, optionally substituted aryl, optionally substituted aryloxy, C1-8 lower alkoxy, optionally substituted aralkyloxy, NR1R2 (wherein R1 and R2 are each as defined above)] or pharmaceutically acceptable acid-addition salts thereof is prepared These compds. are useful as inhibitors of serine protease such as trypsin, chymotrypsin, plasmin, or thrombin and for the treatment of pancreatitis, bleeding, thrombosis, nephritis, and general internal clot and prevention of blood coagulation under perfusion during dialysis or exchange of blood plasma. Thus, 3.44 g DCC was added to a mixture of 3.85 g N,N-dimethylcarbamoylmethyl 2-(4-hydroxyphenyl)propionate,

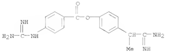
L4 ANSWER 29 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
3.00 g 4-guanidinobenzoic acid hydrochloride, and 20 mL pyridine and the resulting mixt. was stirred at room temp. overnight to give, after workup and acidification with MeSO3H, N,N-dimethylcarbamoylmethyl 2-[4-(4-guanidinobenzoyloxy)phenyl]propionate methanesulfonate, which in vitro showed IC50 of 1.4 + 10-7 and 1.9 + 10-8 M against trypsin and plasmin, resp. A tablet formulation contg. (S)-(+)-I.MeSO3H (A = CH2Ph) was prepd.

IT 159239-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [(guanidinobenzoyloxy)phenyl]propionic acid derivs. as serine protease inhibitors)

RN 159239-63-1 CAPLUS
CN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-(2-amino-2-imino-1-methylethyl)phenyl ester, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

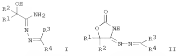
CRN 159239-62-0
CMF C17 H19 N5 O2



CM 2

CRN 75-75-2
CMF C H4 O3 S

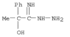
L4 ANSWER 30 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:224478 CAPLUS
DOCUMENT NUMBER: 122:81192
ORIGINAL REFERENCE NO.: 122:15427a,15430a
TITLE: 4-hydrazonooxazolidin-2-ones from ω-substituted glycolamidrazones
AUTHOR(S): Geffken, D.; Holst, C.
CORPORATE SOURCE: Inst. Pharmazie, Universitaet Hamburg, Germany
SOURCE: Pharmazie (1994), 49(11), 821-4
CODEN: PHARAT; ISSN: 0031-7144
PUBLISHER: Govi-Verlag Pharmazeutischer Verlag
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 122:81192
GI



AB Hydrazinolysis of the glycolimidates gave glycolamidrazones which were with acetone or benzaldehyde to give hydrazono derivs. of type 4. I (R1 = alkyl, Ph, etc.; R2 = H, Me; R3 = Me, Ph, etc.; R4 = H, Me). Cyclic carbonylation of I with 1,1'-carbonyldiimidazole yields 4-hydrazono-2-oxazolidinones II (same R1-R4).

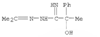
IT 160154-90-5P, α-Hydroxy-α-methylbenzeneethanimidic acid hydrazide 160154-94-9P 160154-97-2P 160154-98-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (hydrazono)xazolidinones from glycolamidrazones)

RN 160154-90-5 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, hydrazide (CA INDEX NAME)

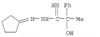


RN 160154-94-9 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, (1-methylethylidene)hydrazide (9CI) (CA INDEX NAME)

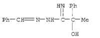
L4 ANSWER 30 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 160154-97-2 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, cyclopentylidenehydrazide (9CI) (CA INDEX NAME)



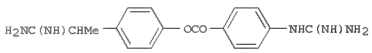
RN 160154-98-3 CAPLUS
CN Benzeneethanimidic acid, α-hydroxy-α-methyl-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)



L4 ANSWER 31 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:692802 CAPLUS
DOCUMENT NUMBER: 121:292802
ORIGINAL REFERENCE NO.: 121:53304h,53305a,53307a
TITLE: Amidinoethyl derivative
INVENTOR(S): Muramatsu, Mutsumi; Tamura, Toshiaki; Yanagi, Toshiji
PATENT ASSIGNEE(S): Teikoku Hormone Mfg Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06228078	A	19940816	JP 1993-305706	19931028
PRIORITY APPLN. INFO.:			JP 1993-305706	19931028

GI



I

AB Amidinoethyl derivative I or its salts are useful as serine protease inhibitors for treatment of diseases (e.g. inflammation, cardiovascular diseases, and pancreatic diseases), caused by abnormalities of the enzyme.
4-(1-Amidinoethyl)phenol methanesulfonic acid salt (preparation given) (5.73 g) was stirred with 5.15 g 4-guanidinobenzoyl chloride HCl salt under ice cooling for 0.5 h and at room temperature overnight to give 3.36 g 4-(1-amidinoethyl)phenyl 4-guanidinobenzoate (II) dimethanesulfonate salt.
II inhibited trypsin and thrombin with IC50 of 3.2 + 10-7 and 6.3 + 10-9 (no unit given).

IT 159239-62-0P 159239-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (amidinoethyl)phenyl guanidinobenzoate for inhibition of serine protease)

RN 159239-62-0 CAPLUS
CN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-(2-amino-2-imino-1-methylethyl)phenyl ester (CA INDEX NAME)

L4 ANSWER 21 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

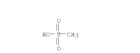
RN 159239-63-1 CAPLUS
CN Benzoic acid, 4-[aminoiminomethyl)amino]-, 4-[2-amino-2-imino-1-methylethyl]phenyl ester, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 159239-62-9
CMF C17 H19 N5 O2

CM 2

CRN 75-75-2
CMF C H4 O3 S



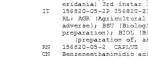
L4 ANSWER 22 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 121:150270
GI

AB The N-arylhydrazine derivs. I [A,B,W=O,CR4;F=halo,CN,NO2,(halo)alkyl,(halo

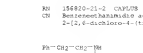
)alkoxy;n=0,1,2;Q=NR2CRO,N:CRX1,N:CR(NR3R4);R=H,(halo)alkyl,cycloalkyl,(ha lo)alkoxy,etc.;R1,R2=H,alkyl;R3,R4=H,(un)substituted alkyl,Ph or pyridyl, etc.] are prepared as acaricides and insecticides. Treatment of 2,6-dichloro-4-(trifluoromethyl)phenylhydrazine with trimethylacetyl chloride, in C1CH2Cl, gave 2,2-dimethylpropionic acid 2-(2,6-dichloro-a,a,a-trifluoro-p-tolyl)hydrazide (I). Lima bean leaves dipped in 500 ppm I were lethal to Southern armyworm (Spodoptera eridania) 3rd instar larvae.

IT 156820-29-2P 156820-21-2P 156820-27-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SYN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as acaricides and insecticides)

RN 156820-29-2 CAPLUS
CN Benzeneethanimidic acid, N-ethyl-a,a-dimethyl-, 2-(2,6-dichloro-4-(trifluoromethyl)phenyl)hydrazide (CA INDEX NAME)



RN 156820-21-2 CAPLUS
CN Benzeneethanimidic acid, a,a-dimethyl-N-(2-phenylethyl)-, 2-(2,6-dichloro-4-(trifluoromethyl)phenyl)hydrazide (CA INDEX NAME)



L4 ANSWER 32 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:502030 CAPLUS
DOCUMENT NUMBER: 121:102030
ORIGINAL REFERENCE NO.: 121:18219a,18222a
TITLE: N-arylhydrazine derivatives as insecticides and acaricides
INVENTOR(S): Furch, Joseph Augustus; Kuhn, David George; Hunt, David Allen; Lew, Albert Chieh; Gromoslajski, Cynthia Emma
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: Eur. Pat. Appl., 76 pp
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

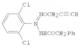
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 604798	A1	19940706	EP 1993-119754	19931208
EP 604798	B1	20040204		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
US 5420165	A	19950530	US 1992-988185	19921229
AT 213387	T	20020315	AT 1993-119754	19931208
ES 2170088	T3	20020716	ES 1993-119754	19931208
CZ 284479	B6	20000412	CZ 1993-2698	19931217
AU 9352679	A	19940714	AU 1993-52679	19931224
AU 675253	B2	19970130		
CA 2112420	C	20070213	CA 1993-2112420	19931224
HU 113556	B1	19980828	HU 1993-1796	19931227
SK 281733	B6	20010710	SK 1993-1484	19931227
IL 108188	A	20011125	IL 1993-108188	19931227
CN 1089938	A	19940727	CN 1993-121610	19931228
CN 1044600	B	19990811		
ZA 9309744	A	19940818	ZA 1993-9744	19931228
JP 06239805	A	19941021	JP 1993-350030	19931228
JP 3816543	B2	20060830		
HR 9305254	A	19941101	HR 1993-5254	19931228
HU 67294	A2	19950228	HU 1993-3772	19931228
HU 221126	B1	20020828		
PL 175499	B1	19990129	PL 1993-317481	19931228
PL 176108	B1	19990430	PL 1993-301659	19931228
RO 2140738	C1	19991110	RO 1993-56949	19931228
CA 2112420	A1	19940630	CA 1994-2112420	19940121
US 5583389	A	19961217	US 1995-431227	19950428
US 5646278	A	19970708	US 1995-431154	19950428
US 5693860	A	19971202	US 1995-439671	19950428
JP 2005263909	A	20050929	JP 2005-134574	20050502
PRIORITY APPLN. INFO.:			US 1992-988185 A	19921229
			US 1992-988194 A	19921229
			US 1992-988195 A	19921229
			JP 1993-350030 A3	19931228

L4 ANSWER 32 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 156820-27-8 CAPLUS
CN Benzeneethanimidic acid, 4-chloro-N-ethyl-a,a-dimethyl-, 2-(2,6-dichloro-4-(trifluoromethyl)phenyl)hydrazide (CA INDEX NAME)

L4 ANSWER 33 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:6034 CAPLUS
DOCUMENT NUMBER: 114:6034
ORIGINAL REFERENCE NO.: 114:1187a,1190a
TITLE: Preparation of N-hydroxyamidines as acaricides and agricultural and horticultural fungicides
INVENTOR(S): Kishimoto, Takashi; Hayakawa, Koichi; Nakayama, Akira; Yamada, Tomio; Takahashi, Eiko; Hashimoto, Akira; Sano, Shinsuke; Hosokawa, Hiroyasu
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02006453	A	19900110	JP 1988-158393	19880627
PRIORITY APPLN. INFO.:			JP 1988-158393	19880627

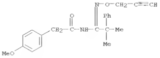
OTHER SOURCE(S): MARPAT 114:6034
GI



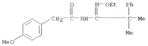
III

AB Amidines R1[R5(R2O)N]C:NR3 (I) and R1(R3R4N)C:NOR2 II [R1 = H, (un)substituted Ph, alkyl optionally substituted by (un)substituted Ph, naphthyl, alkylthio, aralkylthio, (un)substituted NH2, cyclic amino, (un)substituted heterocyclyl; R2 = H, (un)substituted alkyl, alkenyl, alkynyl, XR6, X = CO, CONH, CO2, COCO; R6 = alkyl, (un)substituted alkenyl, Ph, or aralkyl, P(:Y)(OR7)2, Y = O, S, R7 = alkyl; R3 = H, (un)substituted alkyl, alkynyl, ZR8; Z = CO, CS, CO2, COCO, CONH, SO2, O2C; R8 = (un)substituted alkyl, alkenyl, or aralkyl, piperidino; R4 = H, alkyl; R5 = alkyl, aralkyl, (un)substituted aralkylcarbonyl] are prepared, e.g. by reaction of R1C(X):NOR2 (X = halo) with HNR3R4. Thus, PhCH2COCl was added to a solution of 2,6-Cl2C6H3C(NH2):NOCH2C.tplbond.CH in benzene and the mixture was refluxed overnight to give a benzamidine III. A total of 574 II were prepared and 18 II at 125 ppm completely controlled Tetranychus urticae and III and 46 others at 200 ppm controlled 77-100% Erysiphe graminis.
IT 129860-61-3P 129860-62-4P 129860-63-5P

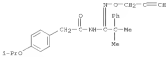
L4 ANSWER 33 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
129860-64-6P 129860-67-9P 129860-68-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of, as acaricide and agrochem. fungicide)
RN 129860-61-3 CAPLUS
CN Benzeneacetamide, 4-methoxy-N-[2-methyl-2-phenyl-1-[(2-propynyloxy)amino]propylidene]- (9CI) (CA INDEX NAME)



RN 129860-62-4 CAPLUS
CN Benzeneacetamide, N-[1-(ethoxyamino)-2-methyl-2-phenylpropylidene]-4-methoxy- (9CI) (CA INDEX NAME)

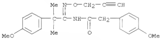


RN 129860-63-5 CAPLUS
CN Benzeneacetamide, 4-(1-methylethoxy)-N-[2-methyl-2-phenyl-1-[(2-propynyloxy)amino]propylidene]- (9CI) (CA INDEX NAME)

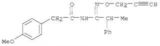


RN 129860-64-6 CAPLUS
CN Benzeneacetamide, 4-methoxy-N-[2-(4-methoxyphenyl)-2-methyl-1-[(2-propynyloxy)amino]propylidene]- (9CI) (CA INDEX NAME)

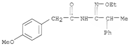
L4 ANSWER 33 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 129860-67-9 CAPLUS
CN Benzeneacetamide, 4-methoxy-N-[2-phenyl-1-[(2-propynyloxy)amino]propylidene]- (9CI) (CA INDEX NAME)



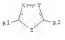
RN 129860-68-0 CAPLUS
CN Benzeneacetamide, N-[1-(ethoxyamino)-2-phenylpropylidene]-4-methoxy- (9CI) (CA INDEX NAME)



L4 ANSWER 34 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:77194 CAPLUS
DOCUMENT NUMBER: 112:77194
ORIGINAL REFERENCE NO.: 112:13203a,13206a
TITLE: Preparation of oxadiazoles as central muscarinic acetylcholine receptor stimulants and pharmaceutical compositions containing them
INVENTOR(S): Baker, Raymond; Merchant, Kevin J.; Saunders, John; Street, Leslie J.
PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 323864	A2	19890712	EP 1989-200001		19890102
EP 323864	A3	19911218			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
ZA 8900045	A	19900926	ZA 1989-45		19890104
DK 8900041	A	19890709	DK 1989-41		19890106
AU 8927798	A	19890720	AU 1989-27798		19890106
AU 628311	B2	19920917			
JP 02149580	A	19900608	JP 1989-571		19890106
PRIORITY APPLN. INFO.:			GB 1988-394	A	19880108
			GB 1988-13513	A	19880608
			GB 1988-24898	A	19881024

GI



I

AB The title compds. [I; R1 = non-aromatic aza(bi)cyclic ring residue, e.g., pyrrolidinyl, piperidinyl, tetrahydropyridinyl; R2 = (substituted) saturated hydrocarbyl, e.g., Pr, Me2CH; one of X, Y, and Z = O and the other 2 = N], central muscarinic acetylcholine receptor stimulants, useful for treatment and prevention of neurodegenerative diseases, are prepared via cyclocondensation of R3CO2H with HON:CR4NH2 or R4CONHNH2 [one of R3 and R4 = non-aromatic aza(bi)cyclic ring residue and the other = (substituted) saturated hydrocarbyl]. PhCH2C(NH2):NOH was condensed with 3-(methoxycarbonyl)quinuclidine in THF containing NaH to give 3-(3-benzyl-1,2,4-oxadiazol-5-yl)quinuclidine, isolated as its

L4 ANSWER 34 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
hemisulfate. A tablet comprising
3-(3-cyclopropyl-1,2,4-oxadiazol-5-yl)-1-
azabicyclo[2.2.1]heptane 1.0, microcryst. cellulose 49.25, modified food
corn starch 49.25, and Mg stearate 0.50 mg was formulated. I had an IC50
of better than 10 μM for displacement of specifically bound
[3H]-N-methylscopolamine from muscarinic receptors of rat cortical
membrane preps.
IT 42131-53-5, 2-Phenylpropionamide oxime
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, in preparation of oxadiazoles for treatment of
neurodegenerative diseases)
RN 42131-53-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl- (CA INDEX NAME)

L4 ANSWER 35 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1981:480429 CAPLUS
DOCUMENT NUMBER: 95:80429
ORIGINAL REFERENCE NO.: 95:11591a,11594a
TITLE: Synthesis and properties of the tremor-inducing N-carbamoylacetamidine derivative LCN-954 and some related compounds
AUTHOR(S): Bream, John D.; Picard, Claude W.; White, Trevor G.
CORPORATE SOURCE: Wander Res. Inst., Wander Ltd., Bern, CH-3001, Switz.
SOURCE: European Journal of Medicinal Chemistry (1981), 16(2), 175-9
CODEN: EJMCA5; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:80429
GI

AB The hydration of N-cyanophenylacetamidines gave N-carbamoyl analogs I (Z = CH2, CHMe, CHCHCH2, OCH2; R1 = H, Cl, Cl2; R2 = H, Me; R3 = H, Me; R4 = H, Me). Thus, 2,6-Cl2C6H3CH2C(:NCN)NH2 was treated with concentrated HCl at 40-50° to give 2,6-Cl2C6H3CH2C(:NCONH2)NH2.HCl. The latter showed tremorogenic activity, while the other prepared I excluded anti-tremorogenic activity.
IT 55769-76-1P 55769-91-0P 78622-01-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-tremorogenic activity of)
RN 55769-76-1 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-2-chloro-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L4 ANSWER 33 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 55769-91-0 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 78622-01-2 CAPLUS
CN Benzeneethanimidamide, N-(aminocarbonyl)-2,6-dichloro-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

IT 55770-09-7P 78622-11-4P 78630-47-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydration of, N-carbamoylamidine analog from)
RN 55770-09-7 CAPLUS
CN Benzeneethanimidamide, 2-chloro-N-cyano-α-methyl- (CA INDEX NAME)

RN 78622-11-4 CAPLUS
CN Benzeneethanimidamide, N-cyano-α-methyl- (CA INDEX NAME)

RN 78630-47-4 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-N-cyano-α-methyl- (CA INDEX

L4 ANSWER 35 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
NAME)

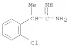
IT 78622-20-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with cyanogen bromide)
RN 78622-20-5 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-α-methyl- (CA INDEX NAME)

IT 78622-19-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of cyanogen bromide with free base from)
RN 78622-19-2 CAPLUS
CN Benzeneethanimidamide, 2,6-dichloro-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

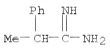
IT 55770-08-6 78622-24-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyanogen bromide)
RN 55770-08-6 CAPLUS
CN Benzeneethanimidamide, 2-chloro-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 35 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● HCl

RN 78622-24-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 36 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:406123 CAPLUS
DOCUMENT NUMBER: 89:6123
ORIGINAL REFERENCE NO.: 89:1043a,1046a
TITLE: O-(3-Amino-2-hydroxypropyl)amidoxime derivatives
INVENTOR(S): Takacs, Kalman; Nagy, Peter Literati; Kiss, Ilona; Simay, Antal; Szentivanyi, Matyas; Virag, Sandor; Farago, Katalin
PATENT ASSIGNEE(S): Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., Hung.
SOURCE: Ger. Offen., 33 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2738589	A1	19780302	DE 1977-2738589	19770826
DE 2738589	C2	19900419		
HU 19948	A2	19810528	HU 1976-CI1682	19760827
HU 177578	B	19811128		
AT 7706054	A	19790815	AT 1977-6054	19770822
AT 355554	B	19800310		
SE 7709482	A	19780228	SE 1977-9482	19770823
SE 435280	B	19840917		
SE 435280	C	19841220		
NL 7709276	A	19780301	NL 1977-9276	19770823
NL 187478	B	19910516		
NL 187478	C	19911016		
IL 52804	A	19810629	IL 1977-52804	19770823
DD 132433	A5	19780927	DD 1977-200719	19770824
CS 204008	B2	19810331	CS 1977-5551	19770824
GB 1582029	A	19801231	GB 1977-35745	19770825
BE 858134	A1	19771216	BE 1977-180447	19770826
DK 7703797	A	19780228	DK 1977-3797	19770826
DK 150196	B	19870105		
DK 150196	C	19870706		
FI 7702551	A	19780228	FI 1977-2551	19770826
FI 68396	B	19850531		
FI 68396	C	19850910		
NO 7702958	A	19780228	NO 1977-2958	19770826
NO 144793	B	19810803		
NO 144793	C	19811111		
FR 2362845	A1	19780324	FR 1977-26070	19770826
FR 2362845	B1	19810109		
JP 53050131	A	19780508	JP 1977-102504	19770826
JP 62016942	B	19870415		
AU 7728254	A	19790301	AU 1977-28254	19770826
AU 521432	B2	19820401		
PL 106317	B1	19791231	PL 1977-200480	19770826
PL 107628	B1	19800229	PL 1977-206476	19770826
SU 730296	A3	19800425	SU 1977-2514754	19770826
CA 1077506	A1	19800513	CA 1977-285529	19770826

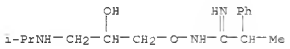
L4 ANSWER 36 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CH 630344	A5	19820615	CH 1977-10473	19770826
US 4187220	A	19800205	US 1977-829148	19770830
CS 204009	B2	19810331	CS 1978-5952	19780914
AT 7808741	A	19800815	AT 1978-8741	19781207
AT 361457	B	19810310		
US 4308399	A	19811229	US 1979-54791	19790705
PRIORITY APPLN. INFO.:			HU 1976-CI1682	A 19760827
			HU 1977-CI1682	A 19770426
			AT 1977-6054	A 19770822
			CS 1977-5551	19770824
			US 1977-829148	A3 19770830

OTHER SOURCE(S): MARPAT 89:6123

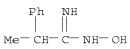
AB RR1NCH2CH(OH)CH2ON:C(NH2)(CHR2)n(CHR3)mR4 I (R = H, C1-5 alkyl; R1 = C1-5 alkyl, cycloalkyl, Ph, optionally substituted by OH or Ph; RR1N = heterocycle; R2 = H, C1-4 alkyl, Ph; R3 = H, C1-4 alkyl, cycloalkyl or Ph, optionally substituted by halogen; R4 = optionally substituted cycloalkyl, aromatic or heterocyclic group; m = n = 0, 1, 2) and their salts were prepared
Thus, PhC(NH2):NOH reacted with 1-chloro-3-piperidino-2-propanol in EtOH to give I (RR1N = piperidino, R4 = Ph, m = n = 0). I are useful as antidiabetics.

IT 66611-55-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66611-55-0 CAPLUS
CN Benzeneethanimidamide, N-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-α-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT 42191-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amines and epichlorohydrin)
RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl- (CA INDEX NAME)



L4 ANSWER 37 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:529660 CAPLUS
DOCUMENT NUMBER: 85:129660
ORIGINAL REFERENCE NO.: 85:17645a,17646a
TITLE: Pyrindine derivatives
INVENTOR(S): Komori, Saburo
PATENT ASSIGNEE(S): Yamagda, Sheoo, Japan
SOURCE: Jpn. Tokkyo Koho, 3 pp.
CODEN: JAXAAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50027673	B	19751204	JP 1970-35552	19700425
PRIORITY APPLN. INFO.:			JP 1970-35552	A 19700425

GI For diagram(s), see printed CA Issue.
AB Anilines I (R, R1 = Cl, alkyl, aralkyl, aryl) were heated with COCl2 to give pyrindilmes II (R2 = Cl, OR). Thus, 2.3 g I (R = Cl, R1 = Me), 2.3 g COCl2, and PhCl were heated 90 hr in a sealed tube at 100-110° to give 2.25 g II (R = R2 = Cl, R1 = Me). Similarly prepared were II (R, R1, R2 given): Cl, Cl, OR; Cl, Ph, Cl; Me, Ph, Cl; Et, Et, Cl.
IT 40645-74-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with phosgene, pyrindine derivative from)
RN 40645-74-9 CAPLUS
CN Benzenesethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

L4 ANSWER 38 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1976:529659 CAPLUS
DOCUMENT NUMBER: 85:129659
ORIGINAL REFERENCE NO.: 85:17645a,17646a
TITLE: Barbituric acid derivatives
INVENTOR(S): Komori, Saburo
PATENT ASSIGNEE(S): Yamagda, Sheoo, Japan
SOURCE: Jpn. Tokkyo Koho, 3 pp.
CODEN: JAXAAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50027673	B	19751204	JP 1970-56192	19700912
PRIORITY APPLN. INFO.:			JP 1970-56192	A 19700912

GI For diagram(s), see printed CA Issue.
AB Nitriles RCH2CN (I) [R, R1 = (substituted) alkyl, Ph] or amides RCH2CONHR2 (II) were treated with COCl2 in the presence of HCl followed by treating the product with H2O to give III, which were also prepared by treating amidines IV (a mixture of cis and trans isomers) [R2, R3 = (substituted) alkyl, Ph] with COCl2 and then with H2O. Thus, 1.5 g IV.HCl (R = R1 = Me) and 2.4 g COCl2 in PhCl were heated in a sealed tube 30 hr at 100-110° to give 0.27 g III (R = R1 = Me), which was also prepared by heating a mixture of isobutyronitrile, HCl, COCl2 and PhCl in a sealed tube 77 hr at 100-110°. Similarly prepared were III (R, R1 given): Me, Et; Me, Ph; Bu, CHClCH2Br; Et, m-ClNC6H4.
IT 40645-76-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with phosgene)
RN 40645-76-9 CAPLUS
CN Benzenesethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

L4 ANSWER 39 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1974:70902 CAPLUS
DOCUMENT NUMBER: 84:70902
ORIGINAL REFERENCE NO.: 84:5043a,5048a
TITLE: Substituted ω-phenylalkanoylbenzoic acids and their functional acid derivatives
INVENTOR(S): Roszs, Alberto
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Patentschrift (Switz.), 6 pp. Division of Swiss 559,173.
CODEN: SWXXA5
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 566311	A5	19750915	CH 1971-13160	19690605
PRIORITY APPLN. INFO.:			CH 1971-13160	19690605

GI For diagram(s), see printed CA Issue.
AB 4-[2-(1-carboxyethyl)phenyl]-5-(methylamino)valeric acid, prepared from 1-methyl-2-oxo-5-[p-(1-chlorethyl)phenyl]pyrrolidine by treatment with NaCN, hydrolysis, and ring cleavage, was cyclized to give the paperazinone I. Antiinflammatory I was effective on rat paws in the Kaolin edema test an oral doses of 30-100 mg/kg.
IT 41789-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41789-12-2 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α-methyl-4-(1-methyl-6-oxo-3-paperazinyl)- (CA INDEX NAME)

L4 ANSWER 40 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1975:115896 CAPLUS
DOCUMENT NUMBER: 82:115896
ORIGINAL REFERENCE NO.: 82:18865a,18868a
TITLE: Acalphatic acetamidines
INVENTOR(S): Ream, John B.
PATENT ASSIGNEE(S): Dr. A. Wander, A.-G., Switz.
SOURCE: Ger. Offen., 28 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2439299	A1	19750306	DE 1974-2439299	19740816
FR 2241300	A1	19750321	FR 1974-27773	19740809
FI 7402392	A	19750221	FI 1974-2392	19740816
NO 7402987	A	19750221	NO 1974-2987	19740812
SE 7410281	A	19750221	SE 1974-10281	19740812
DK 7404280	A	19750428	DK 1974-4280	19740812
NL 7410987	A	19750224	NL 1974-10987	19740816
DD 116606E	A5	19751205	DD 1974-180552	19740816
BE 818988	A1	19750219	BE 1974-147735	19740819
JP 50052043	A	19750509	JP 1974-94329	19740819
AU 7472496	A	19760219	AU 1974-72496	19740819
AT 7406340	A	19760331	AT 1974-6340	19740820
PRIORITY APPLN. INFO.:			GB 1973-39263	A 19730820
			GB 1973-44372	A 19730921

AB Thirty-three RnC6H5-nXC(:NR1)NHCOMR2R3 (Rn = e.g. 3,4-Cl2, 3,4-Me2, 2-Cl, or 3-CF3; X = CH2, CHMe, or CHCHCH3; R1-R3 = H or Me; useful as antidepressants, were prepared by hydrolysis of RnC6H5-nXC(:NR1)NHCN or R2R3NCOCl.
IT 55770-08-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of)
RN 55770-08-6 CAPLUS
CN Benzeneethanimidamide, 2-chloro-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L4 ANSWER 40 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
IT 55769-69-79
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 55769-69-7 CAPLUS
CN Benzeneethanimidamide, 2-chloro-N-cyano-a-methyl- (CA INDEX NAME)

IT 55769-76-1P 55769-81-8P 55769-91-9P
55769-95-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for antihypertensants)
RN 55769-76-1 CAPLUS
CN Benzeneethanimidamide, N-[aminocarbonyl)-2-chloro-a-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 55769-81-8 CAPLUS
CN Benzeneethanimidamide, N-[aminocarbonyl)-3,4-dichloro-a-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 40 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

● HCl

RN 55769-91-9 CAPLUS
CN Benzeneethanimidamide, N-[aminocarbonyl)-a-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 55769-95-4 CAPLUS
CN Benzeneethanimidamide, N-[aminocarbonyl)-3,4-dimethoxy-a-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L4 ANSWER 41 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:464039 CAPLUS
DOCUMENT NUMBER: 79:64039
ORIGINAL REFERENCE NO.: 79:10067a,10070a
TITLE: Aromatic acetamidoxime O-carbamates
INVENTOR(S): Henderson, Rosetta M.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co.
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3742056	A	19730626	US 1971-135806	19710420
PRIORITY APPLN. INFO.:			US 1971-135806	A 19710420

AB Antihypertensive and antiinflammatory acetamidoxime O-carbanates, RnC6H5-nCH(CH3)C(NH2):NO2CONHR2 [Rn = H, 4-Cl, 4-F, 2-Me, 4-MeO, 3,4-(MeO)2, 3,4-Me2, 2,4,6-Me3; R1 = H, Me; R2 = Me, Et] were prepared by treating the acetamidoximes RnC6H5-nCHR1C(NH2):NOH with the isocyanates R2NCO.
IT 42191-44-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42191-44-6 CAPLUS
CN Benzeneethanimidamide, a-methyl-N-[[(methylamino)carbonyl]oxy]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

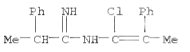
IT 42191-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alkyl isocyanates)
RN 42191-51-5 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-a-methyl- (CA INDEX NAME)

L4 ANSWER 42 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:418585 CAPLUS
DOCUMENT NUMBER: 79:18585
ORIGINAL REFERENCE NO.: 79:2983a,2986a
TITLE: Substituted a-phenylcarboxylicacids
INVENTOR(S): Rossi, Alessio
PATENT ASSIGNEE(S): Ciba-Geigy A.-G.
SOURCE: Patentschrift (Beltz.), 7 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 534690	A	19730430	CH 1972-3553	19690605
PRIORITY APPLN. INFO.:			CH 1972-3553	A 19690605

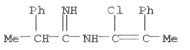
GI For diagram(s), see printed CA Issue.
AB The piperidinylphenylpropionic acids 3 [R = 1-acetyl-2(or 4)-piperidinyl, 1-methyl-2-oxo-4(or 5, or 6)-piperidinyl; R1 = H, Et] were prepared. Thus 4-[4-piperidinyl]phenylacetic acid was acetylated and then methylated with
BuLi-MeI to 2 (R = 1-acetyl-4-piperidinyl, R1 = H). I were antiinflammatory at 30-100 mg/kg orally in the rat paw edema test.
IT 41789-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41789-12-2 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-a-methyl-4-(1-methyl-6-oxo-3-piperidinyl)- (CA INDEX NAME)

L4 ANSWER 43 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:110501 CAPLUS
DOCUMENT NUMBER: 78:110501
ORIGINAL REFERENCE NO.: 78:17743a,17746a
TITLE: Nitrile salts. I. Dimerization of nitriles having α-hydrogen in the presence of hydrogen chloride
AUTHOR(S): Yanagida, Shozo; Fujita, Tetsuo; Ohoka, Masataka; Katagiri, Ichiro; Komori, Saburo
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(1), 292-9
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The compns. and structures of several stable nitrile HCl salts were investigated. Most were dimers and had the structure H2N+:C(CHRR2)NHCCl:CRR1.Cl-; hydrolysis gave HN(CONHRR1)2.
IT 40645-76-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 40645-76-9 CAPLUS
CN Benzeneethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

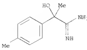
L4 ANSWER 44 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:97594 CAPLUS
DOCUMENT NUMBER: 78:97594
ORIGINAL REFERENCE NO.: 78:15663a,15666a
TITLE: Nitrile salts. II. Facile one-step synthesis of the pyrimidine nucleus
AUTHOR(S): Yanagida, Shozo; Fujita, Tetsuo; Ohoka, Masataka; Kumagai, Reiji; Komori, Saburo
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(1), 299-302
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The reaction of N-(α-chloroalkenyl)alkylamidine hydrochlorides (I) prepared from nitriles with two α-hydrogens reacted with COCl2 at 100-105° to give good yields of 4,6-dichloro-2,5-disubstituted-pyrimidines (II). I, which were obtained from nitriles with only one α-hydrogen, afforded 2-alkylidene-4,6-dichloro-5,5-disubstituted-2,5-dihydropyrimidines (III) in good yields.
IT 40645-76-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phosgene, pyrimidines by)
RN 40645-76-9 CAPLUS
CN Benzeneethanimidamide, N-(1-chloro-2-phenyl-1-propen-1-yl)-α-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L4 ANSWER 45 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1973:84378 CAPLUS
DOCUMENT NUMBER: 78:84378
ORIGINAL REFERENCE NO.: 78:13469a,13472a
TITLE: Meso, racemic, and optically active forms of 3,6-bis[1-hydroxy-1-(4-methylphenylethyl]-1,2,4,5-tetrazines and related systems along with the corresponding 3,5-disubstituted 1,2,4-triazoles, their 4-amino derivatives, and 2,5-disubstituted 1,3,4-oxadiazoles including their circular dichroism spectra
AUTHOR(S): Neilson, D. G.; Mahmood, Safia; Watson, K. M.
CORPORATE SOURCE: Dep. Chem., Univ. Dundee, Dundee, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), (4), 335-9
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 78:84378
GI For diagram(s), see printed CA Issue.
AB (±)-, (+)-, (-)-, and meso-3,6-bis[1-hydroxy-1-(4-methylphenyl)-ethyl]-1,2,4,5-tetrazine (I) were prepared from the appropriate amidinium chlorides and H2NNH2.H2O. Reduction of I gave the corresponding 1,2-dihydrotetrazines (II) which rearranged in HCl-MeOH to give 4-amino-1,2,4-triazoles (III). Deamination of III with HNO2 gave 3,5-bis[1-hydroxy-1-(4-methylphenyl)ethyl]-1,2,4-triazoles. A mixture of meso- and (±)-I with MeCO3H gave 2,5-bis[1-hydroxy-1-(4-methylphenyl)ethyl]-1,3,4-oxadiazole. The 1-hydroxy-1-phenylethyl and 1-hydroxy-1-phenylpropyl analogs of I and II underwent similar reactions. The optically active compds. were studied by CD.
IT 941-50-4 941-51-5 941-52-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of)
RN 941-50-4 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

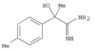
Rotation (+).



● HCl

RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-,

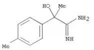
L4 ANSWER 45 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



● HCl

L4 ANSWER 46 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:405728 CAPLUS
DOCUMENT NUMBER: 75:5728
ORIGINAL REFERENCE NO.: 75:951a,954a
TITLE: α-Phenyl carboxylic acid compounds
INVENTOR(S): Rossi, Alberto
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: Ger. Offen., 98 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

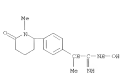
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2025518	A	19701210	DE 1970-2025518		19700526
CH 559173	A5	19750228	CH 1969-8650		19690605
CH 573909	A5	19760331	CH 1970-6221		19700424
CA 980783	A1	19751230	CA 1970-83721		19700526
US 3801581	A	19740402	US 1970-41107		19700527
ZA 7003642	A	19710127	ZA 1970-3642		19700528
FR 2052932	A1	19710416	FR 1970-20213		19700602
FR 2052932	A5	19710416			
ES 380333	A1	19720916	ES 1970-380333		19700603
BE 751451	A	19701204	BE 1970-751451		19700604
NL 7008158	A	19701208	NL 1970-8158		19700604
GB 1319251	A	19730606	GB 1970-27284		19700605
GB 1319252	A	19730606	GB 1972-55884		19700605
US 3853892	A	19741210	US 1973-338698		19730307
PRIORITY APPLN. INFO.:			CH 1969-8650	A	19690605
			CH 1969-18441	A	19691211
			CH 1970-6221	A	19700424
			CH 1969-6221	A	19700424
			US 1970-41107	A2	19700527

AB Title compds., useful as anti-inflammatory agents, have the structure AC6H4CR1R2X, in which A = azacycloalkyl or -alkenyl, R1 and R2 are H or alkyl, and X = CO2H or a derivative Thus, 4-phenylpiperidine treated with C5H5N and AcCl give 1-acetyl-4-phenylpiperidine (I). I, AcCl, and CS2 is treated with AlCl3 to give 1-acetyl-4-(p-acetylphenyl)piperidine (II). II reduced with NaBH4 gives 1-acetyl-4-[p-(1-hydroxyethyl)phenyl]piperidine (III). SOCl2 converts III into 1-acetyl-4-[p-(1-chloroethyl)phenyl]piperidine, which is treated with NaCN to give 1-acetyl-4-[p-(1-cyanoethyl)phenyl]piperidine (IV). IV and aqueous ethanolic KOH, then HCl gives the HCl salt of α-[p-(4-piperidyl)phenyl]propionic acid, which is converted to its Et ester (V), then acetylated to give ethyl α-[p-(1-acetyl-4-

L4 ANSWER 46 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

piperidyl)phenyl]propionate, hydrolysis of which gives α-[p-(1-acetyl-4-piperidyl)phenyl]propionic acid. IV was similarly prepd. from 2-(p-bromophenyl)-2-methyl-1,3-dioxolane Grignard reagent and 1-benzyl-4-piperidone via 2-[p-(1-benzyl-4-hydroxy-4-piperidyl)phenyl]-2-methyl-1,3-dioxolane, p-(1-benzyl-1,2,5,6-tetrahydro-4-pyridyl)acetophenone, and 1-hydroxy-1-[p-(4-piperidyl)phenyl]ethane. 1-Methyl-2-oxo-5-[p-(1-cyanoethyl)phenyl]piperidine is treated with NH2OH.HCl to give α-[p-(1-methyl-2-oxo-5-piperidyl)phenyl]propionamidoxime. p-(1-Acetyl-4-piperidyl)acetophenone, morpholine, and S react to give p-(1-acetyl-4-piperidyl)phenylthioacetic acid morpholide, which is hydrolyzed to p-(4-piperidyl)phenylacetic acid-HCl.

IT 32262-02-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 32262-02-5 CAPLUS
CN Hydratropamidine, N-hydroxy-p-(1-methyl-6-oxo-3-piperidyl)- (8CI) (CA INDEX NAME)



L4 ANSWER 47 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

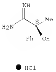
ACCESSION NUMBER: 1969:42424 CAPLUS
DOCUMENT NUMBER: 70:42424
ORIGINAL REFERENCE NO.: 70:7973a,7976a
TITLE: Optical rotatory dispersion of α-hydroxy amidines and their transition metal complexes
AUTHOR(S): Neilson, Douglas G.
CORPORATE SOURCE: Univ. St. Andrews, Dundee, UK
SOURCE: Some Newer Phys. Methods Struct. Chem.; Proc. Symp. (1967), Meeting Date 1966, 186-91. Editor(s): Bonnett, R. United Trade Press Ltd.: London, Engl.
CODEN: 20LHA8
DOCUMENT TYPE: Conference
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB O.R.D. of mandelamidinium chlorides (I) and lactamidinium chloride (II) were measured in MeOH or H2O to obtain their absolute configuration, but the results were rather irregular: no full Cotton effect curves could be measured for (-)-I [R = H, 2-Cl, and 2-Br] and (-)-II, while 2 extrema were observed for (+)-I [2-MeO, 2-EtO, 4-MeO and 4-EtO]. Thus, O.R.D. of the Cu complexes were measured: all the Cu complexes of α-hydroxyamidines of known D-configuration exhibited a pos. Cotton effect, which permitted the D-configuration to be assigned to I [2-MeO, 2-EtO, 2-Cl, 2-Br, 4-MeO, 4-EtO, 3-EtO and 2,4-di-Cl] for which chemical methods cannot be applied owing to the facile racemization. The Cu complex of D-(+)-II gave a pos. O.R.D. curve, establishing the greater value of O.R.D. curves of Cu complexes over that of the parent amidines for the correlation of configuration. The Ni complex is also effective but proved difficult to synthesize. O.R.D. curves of some of the Cu complexes of I [2-EtO, 3-EtO and 4-MeO] have an addnl. extrema near 270 mμ. The Cotton effect owing to the ligand is counterbalanced by an effect of opposite sign but approx. equal intensity owing to the complex as a whole. Support for this argument was given by comparing the circular dichroism curves of I [2-Cl] and I [2-EtO] and their Cu complexes. O.R.D. of compds. containing the amidine group in a heterocyclic ring (e.g., imidazoline) are also discussed.

IT 22210-97-5
RL: PROC (Process)
(optical rotary dispersion of)
RN 22210-97-5 CAPLUS
CN Mandelamidine, α-methyl-, monohydrochloride, (+)- (8CI) (CA INDEX NAME)

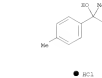
Absolute stereochemistry.



L4 ANSWER 47 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L4 ANSWER 48 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:454040 CAPLUS
DOCUMENT NUMBER: 63:54040
ORIGINAL REFERENCE NO.: 63:9784a-c
TITLE: Optical rotatory dispersion. XIX. A series of acids, imidazolines, amidinium chlorides, and their copper complexes, related to mandelic acid
AUTHOR(S): Emerson, T. R.; Ewing, D. F.; Klyne, W.; Neilson, D. G.; Peters, D. A. V.; Roath, L. R.; Swan, E. J.
CORPORATE SOURCE: Univ. London, Swed.
SOURCE: Journal of the Chemical Society (1965), (July), 4007-14
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The optical rotatory dispersion (o.r.d.) curves of series of α-hydroxy acids related to mandelic acid show that the Cotton-effect curves observed are generally due to the n → π* transition of the carboxyl group and not to the phenyl absorption band (240-280 mμ). The o.r.d. curves for the related amidinium chlorides show distinct extrema in the 250-280 mμ region when the phenyl group carries an alkoxy-substituent. The o.r.d. curves of the amidinium chlorides, however, are more complex than those of their parent acids and not so useful for configurational assignments. Cu complexes derived from these α-hydroxyamidinium chlorides show a Cotton effect at ~appx.590 mμ. Compds. of D-configuration have a positive Cotton effect in this region. This rule has permitted the assignment of configuration to some 10 amidines, not previously correlated by chemical means.
IT 941-52-6 92442-87-0
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

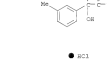
Rotation (-).



● HCl

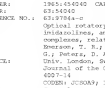
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 48 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CN Mandelamidine, α,4-dimethyl-, hydrochloride (7CI) (CA INDEX NAME)



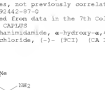
● HCl

L4 ANSWER 48 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● HCl

IT 941-51-5, Mandelamidine, p,α-dimethyl-, hydrochloride, D-(-)- 4023-95-4, Mandelamidine, α-methyl-, hydrochloride, D-(-)- 94281-37-5, Mandelamidine, m,α-dimethyl-, hydrochloride, D-(-)-
(optical rotatory dispersion and spectrum of)
RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 4023-95-4 CAPLUS
CN Mandelamidine, α-methyl-, hydrochloride, D-(-)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 94281-37-5 CAPLUS

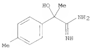
L4 ANSWER 49 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:454039 CAPLUS
DOCUMENT NUMBER: 63:54039
ORIGINAL REFERENCE NO.: 63:9785h,9784a
TITLE: Optical rotatory dispersion. XV. Monosubstituted succinic acids
AUTHOR(S): Fredga, A.; Jennings, J. P.; Klyne, W.; Scopes, Patricia M.; Sjoberg, B.; Sjoberg, S.
CORPORATE SOURCE: Univ. Uppsala, Swed.
SOURCE: Journal of the Chemical Society (1965), (July), 3928-33
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 62, 13191b; 63, 7065g. The ORD curves of many α-substituted succinic acids are measured. All these compds. show Cotton effects associated with the carboxyl absorption band at about 225 mμ. α-Alkyl-, α-aryl-, and α-halosuccinic acids of the D-configuration all give pos. Cotton effects in water and in MeOH; D-α-alkylthiosuccinic acids give somewhat more complex pos. curves. D-α-Hydroxysuccinic acid (D-malic acid) and its O-alkyl ethers give neg. Cotton effects in water and in MeOH. The signs of the dispersion curves of most of these acids are reversed on the addition of alkali.
IT 941-51-5 941-52-6 92442-87-0
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

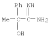
Rotation (-).

L4 ANSWER 49 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● HCl

RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 50 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1965:66553 CAPLUS
DOCUMENT NUMBER: 62:66553
ORIGINAL REFERENCE NO.: 62:11821e-h,11822a-e
TITLE: 1,2,4-Oxadiazoles with pharmaceutical effect
INVENTOR(S): Harsanyi, Kalman; Kiss, Pal; Korbonits, Dezso; Malyata, Ilona; Erdelyi, Ilona; Tardos, Laszlo; Leszkovszky, Gyorgy
PATENT ASSIGNEE(S): Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt.
SOURCE: 23 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 151748		19641223	HU	19630329
BE 645822			BE	
NL 302339			NL	
US 3280122		19661018	US 1964-354465	19640324
PRIORITY APPLN. INFO.:			HU	19630329

OTHER SOURCE(S): MARPAT 62:66553

AB A mixture of 24 g. β,β-diphenylpropionamidoxime(I), 37 g. Et β-piperidinopropionate, 200 ml. absolute EtOH, and 2.3 g. Na is refluxed 8 hrs., concentrated in vacuo, 200 ml. H2O and 4.0 g. NaOH are added, and the mixture is extracted with C6H6. The organic phase is concentrated in vacuo and treated with 100 ml. EtOH-HCl to precipitate 29.22 g. 3-(β,β-diphenylethyl)-5-(β-piperidinoethyl)-1,2,4-oxadiazole-HCl, m. 192-3° (EtOH). Similarly are prepared the following derivs.: 3-(β,β-diphenylethyl)-5-(β-pyrrolidinoethyl)-1,2,4-oxadiazole H maleate, m. 129-31° (H2O or EtOAc), 3-(β,β-diphenylethyl)-5-piperidinomethyl-1,2,4-oxadiazole-HCl, m. 188-9°, 3-(β,β-diphenylethyl)-5-(β-diethylaminoethyl)-1,2,4-oxadiazole-HCl, m. 181°, 3-(β,β-diphenylethyl)-5-(4-aminophenyl)-1,2,4-oxadiazole, m. 149° (96% EtOH), 3-(β,β-diphenylethyl)-5-(4-pyridyl)-1,2,4-oxadiazole, m. 158-9°, 3-(β,β-diphenylethyl)-5-(3-pyridyl)-1,2,4-oxadiazole, m. 137°, 3-(β,β-diphenylethyl)-5-(2-pyridyl)-1,2,4-oxadiazole, m. 151-2°, 3-(α,β-diphenylethyl)-5-piperidinomethyl-1,2,4-oxadiazole-HCl, m. 185°, 3-diphenylmethyl-5-piperidinomethyl-1,2,4-oxadiazole-HCl, m. 161°, 3-diphenylmethyl-5-(β-piperidinoethyl)-1,2,4-oxadiazole-HCl, m. 197°, 3-(3,4-dimethoxybenzyl)-5-(β-morpholinoethyl)-1,2,4-oxadiazole-HCl, m. 181°, 3-(3,4-dimethoxybenzyl)-5-(β-pyrrolidinoethyl)-1,2,4-oxadiazole-HCl, m. 162°, 3-(3,4-dimethoxybenzyl)-5-(β-piperidinoethyl)-1,2,4-oxadiazole-HCl, m. 177°, 3-(3,4-dimethoxybenzyl)-5-piperidinomethyl-1,2,4-oxadiazole-HCl, m. 189°, 3-benzyl-5-(β-morpholinoethyl)-1,2,4-oxadiazole-HCl, m. 173°, 3-benzyl-5-(β-pyrrolidinoethyl)-1,2,4-oxadiazole-HCl, m. 156°, 3-(p-chlorobenzyl)-5-(β-piperidinoethyl)-1,2,4-oxadiazole-HCl, m. 183°,

L4 ANSWER 50 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

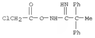
3-(p-chlorobenzyl)-5-(β-morpholinoethyl)-1,2,4-oxadiazole-HCl, m. 179-80°, 3-(p-chlorobenzyl)-5-piperidinomethyl)-1,2,4-oxadiazole-HCl, m. 157°, 3-(p-chlorobenzyl)-5-(β-pyrrolidinoethyl)-1,2,4-oxadiazole-HCl, m. 155°, 3-[β,β-bis(4-chlorophenyl)ethyl]-5-piperidinomethyl-1,2,4-oxadiazole H maleate, m. 117°, 3-(β,β-bis(4-chlorophenyl)ethyl-5-(β-piperidinoethyl)-1,2,4-oxadiazole H maleate, m. 126°, 3-[bis(3,4-dimethoxyphenyl)methyl]-5-(β-piperidinoethyl)-1,2,4-oxadiazole, m. 94° (abs. EtOH), 3-[bis(3,4-dimethoxyphenyl)methyl]-5-(β-morpholinoethyl)-1,2,4-oxadiazole, m. 112-13° (abs. EtOH), 3-(α,β-diphenylethyl)-5-(β-piperidinoethyl)-1,2,4-oxadiazole-HCl, m. 186-7° (abs. EtOH), 3-(α,β-diphenylethyl)-5-[β-(N-methylpiperazino)ethyl]-1,2,4-oxadiazole-2HCl, m. 191° (96% EtOH), 3-(β,β-diphenylethyl)-5-[β-(N-methylpiperazino)ethyl]-1,2,4-oxadiazole, m. 83° [dihydrochloride m. 205-7° (96% EtOH)], 3-diphenylmethyl-5-[β-(N-methylpiperazino)ethyl]-1,2,4-oxadiazole, m. 97° [dihydrochloride m. 196° (96% EtOH)], 3-(p-chlorobenzyl)-5-[β-(N-methylpiperazino) ethyl]-1,2,4-oxadiazole-2HCl, m. 186.5-8.5° (96% EtOH), 3-[bis(3,4-dimethoxyphenyl)methyl]-5-[β-(N-methylpiperazino) ethyl]-1,2,4-oxadiazole-2HCl, m. 219-21° (96% EtOH), and 3-(3,4-dimethoxybenzyl)-5-[β-(N-methylpiperazino) ethyl]-1,2,4-oxadiazole-2HCl, m. 191-3° (96% EtOH). A mixt. of 84 g. I in 1310 ml. C6H6 and 24.53 g. γ-chlorobutyryl chloride in 170 ml. C6H6 is kept at room temp. 24 hrs. and filtered, the solid suspended in 1000 ml. H2O, and the mixt. kept 24 hrs. and filtered to give 44.59 g. O-γ-chlorobutyryl-β,β-diphenylpropionamidoxime (II), m. 145°. II (10.35 g.) and Ac2O (6 ml.) heated on a water-bath, treated with H2O and C6H6, and the org. phase washed with Na2CO3 soln. and concd. gives 9.90 g. 3-(β,β-diphenylethyl)-5-(γ-chloropropyl)-1,2,4-oxadiazole (III) (m.p. not given). A mixt. of 9.90 g. III, 45 ml. PhMe, and 8.90 ml. piperidine is refluxed 11 hrs. and filtered and the filtrate washed with H2O and evapd. to yield 11.20 g. 3-(β,β-diphenylethyl)-5-(γ-piperidinopropyl)-1,2,4-oxadiazole. H maleate m. 146-7° (Me2CO). The γ-morpholinopropyl deriv. is prepd. similarly, H maleate m. 153°. A soln. of 14.53 g. β-chloropropionyl chloride in Me2CO is added dropwise with stirring at 0-5° to a suspension of 27.6 g. I and 9.86 g. NaHCO3 in 140 ml. abs. Me2CO and the whole stirred 7 hrs. and added to 1100 ml. H2O to yield 27.8 g. O-(β-chloropropionyl)-β,β-diphenylpropionamidoxime (IV), m. 116-17° (abs. EtOH or C6H6). A soln. of 4.55 g. IV in 25 ml. abs. PhMe and 3 ml. piperidine is refluxed 7 hrs., 20 ml. H2O added, the mixt. evapd. to dryness in vacuo, and the residue treated with HCl in EtOH to give 2.15 g. 3-(β,β-diphenylethyl)-5-(β-piperidinoethyl)-1,2,4-oxadiazole-HCl, m. 192° (abs. EtOH). O-Chloroacetyl-β,β-diphenylpropionamidoxime, m. 118-19° (obtained similarly to IV), is heated in vacuo at 100-10° 10-15 min. to yield 3-(β,β-diphenylethyl)-5-chloromethyl-1,2,4-oxadiazole, m. 73-4° (MeOH). Heating it with piperidine in PhMe and treating the product with HCl in EtOH yields 3-(β,β-diphenylethyl)-5-(piperidinomethyl)-1,2,4-oxadiazole-HCl, m. 187-9° (MeOH). β-Piperidinopropionic acid-HCl (1.97 g.) is added to 2.4 g. I in 20 ml. abs. C5H5N at 20°, the mixt. refluxed 2 hrs. and evapd. to dryness in vacuo, the residue in 10 ml. 2N NaOH extd. with Et2O, the org. phase concd., and the residue treated with HCl in EtOH to ppt. 3-(β,β-diphenylethyl)-5-(β-piperidinoethyl)-1,2,4-

L4 ANSWER 50 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

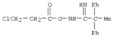
oxadiazole-2HCl, m. 192-3°. These products showed spasmolytic, local anesthetic, cough-reliever, analgesic, anti-inflammatory, antipyretic, and circulation influencing effects.

IT 968-45-6P, Propionamidoxime, 2,2-diphenyl-, O-chloroacetate
971-95-9P, Propionamidoxime, 2,2-diphenyl-, O-3-chloropropionate
974-34-5P, Propionamidoxime, 2,2-diphenyl-, O-4-chlorobutyrate
RL: PREP (Preparation)
(preparation of)

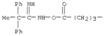
RN 968-45-6 CAPLUS
CN Propionamidoxime, O-(2-chloroacetyl)-2,2-diphenyl-, O-chloroacetate (8CI) (CA INDEX NAME)



RN 971-95-9 CAPLUS
CN Propionamidoxime, 2,2-diphenyl-, O-(3-chloropropionyl)- (8CI) (CA INDEX NAME)



RN 974-34-5 CAPLUS
CN Propionamidoxime, O-(4-chlorobutyryl)-2,2-diphenyl- (8CI) (CA INDEX NAME)



L4 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:76364 CAPLUS
DOCUMENT NUMBER: 62:76364
ORIGINAL REFERENCE NO.: 62:14376f
TITLE: The resolution of some substituted lactamidines and stirolactamidines by means of the mandelic acids
AUTHOR(S): Ewing, D. F.; Neilson, D. G.
CORPORATE SOURCE: Univ. St. Andrews, Dundee, UK
SOURCE: Journal of the Chemical Society [1965], (Jan.), 770-4
CODEN: JCSOAP; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: English
AB p- and p-Methylatrolactamidines were prepared from the corresponding methylacetophenones and were resolved by means of the mandelic acids. o-Methylacetophenone failed to give an amidine. α-Benzyl-lactamidine was also resolved by means of these acids but β-benzyllactamidine showed no separation of the diastereoisomers.
IT 941-50-4 941-52-6 943-23-7 971-52-8
971-57-9
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-50-4 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (±)- (9CI) (CA INDEX NAME)

Rotation (±).

● HCl

RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

L4 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 37199-29-0
CMF C8 H8 O3

Absolute stereochemistry. Rotation (+).

RN 971-53-9 CAPLUS
CN Mandelic acid, (S)-, compd. with (+)-p,α-dimethylmandelamidine (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 46147-67-3
CMF C10 H14 N2 O

Rotation (+).

CM 2

CRN 611-71-2
CMF C8 H8 O3

Absolute stereochemistry. Rotation (-).

L4 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

● HCl

RN 943-23-7 CAPLUS
CN Mandelamidine, α,α-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 971-52-8 CAPLUS
CN Mandelic acid, (S)-, compd. with (-)-α-hydroxy-α-methylhydratropamidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 53623-24-8
CMF C10 H14 N2 O

Rotation (-).

L4 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

IT 109595-37-1, Mandelamidine, α-methyl-
(derive., resolution by mandelic acids)
RN 109595-37-1 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl- (CA INDEX NAME)

IT 941-53-5P, Mandelamidine, p,α-dimethyl-, hydrochlorid, isomers 94281-37-5P, Mandelamidine, m,α-dimethyl-, hydrochloride, isomers 95157-78-8P, Mandelic acid, compound with m,α-dimethylmandelamidine (1:1), (+)- 95157-78-1P, Mandelic acid, compound with p,α-dimethylmandelamidine (1:1), isomers
RL: PREP (Preparation)
(preparation of)
RN 941-53-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 94281-37-5 CAPLUS
CN Mandelamidine, m,α-dimethyl-, hydrochloride (7CI) (CA INDEX NAME)

L4 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

● HCl

RN 95157-76-9 CAPLUS
CN Mandelic acid, compd. with α,α-dimethylmandelamidine (7CI) (CA INDEX NAME)

CM 1

CRN 95157-75-8
CMF C10 H14 N2 O

CM 2

CRN 90-64-2
CMF C8 H8 O3

RN 95157-78-1 CAPLUS
CN Mandelic acid, compd. with β,α-dimethylmandelamidine (7CI) (CA INDEX NAME)

CM 1

CRN 95157-77-0
CMF C10 H14 N2 O

L4 ANSWER 51 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 90-64-2
CMF C8 H8 O3

L4 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1965:36363 CAPLUS
DOCUMENT NUMBER: 62:36363
ORIGINAL REFERENCE NO.: 62:6374e-f
TITLE: Electrophilic substitution at saturated carbon. XXIV. Trifluoromethyl as a carbanion-stabilizing group
AUTHOR(S): Cram, Donald J.; Wingrove, Alan S.
SOURCE: Journal of the American Chemical Society (1964), 86(24), 5490-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two systems have been prepared for study of the stereochem. course of the base-catalyzed β-O exchange at C attached to a trifluoromethyl group. Optically active 2-methyl-3-phenyl-1,1,1-trifluoropropane (I) and the same compound deuterated in the 2-position, and optically active 2-phenyl-1,1,1-trifluoroborneol (II) and its deuterated counterpart (2-position) were examined. In tert-BuOD at 124°, (+)-I was found to undergo elimination reaction to the exclusion of isotopic exchange. The initially formed 1,1-difluoro-2-methyl-3-phenyl-1-propene underwent a base-catalyzed allylic rearrangement to give a 6.5:1 mixture of trans- to cis-3,3-difluoro-2-methyl-1-phenyl-1-propene (trans- to cis-III), which were identified by their spectral properties. The base-catalyzed elimination reaction exhibited a kinetic isotope effect of 3.2, a fact which suggests a carbanion intermediate for the reaction. II also underwent elimination to give 1,1-difluoro-2-phenyl-1-butene and its geometers. However, β-D exchange also occurred, but at a much slower rate. In tert-BuOH-tert-BuCF3 and in EtOH-KOEt, isotopic exchange went with total racemization (ke/kx, the ratio of the rate constant for exchange to the rate constant for racemization, was equal to unity). In MeOH-KOMe, or MeOH-MeCl3, isotopic exchange went with net inversion (ke/kx, ranged from 0.69 to 0.84, depending on whether the substrate or the solvent was D labeled). This result is interpreted in terms of an asym.-solvated syn. and dissociated carbanion.
IT 941-50-4 941-51-5 941-52-6 943-23-7
971-32-8 971-33-9 9428-27-5
95157-76-7
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 941-50-4 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

● HCl

L4 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 941-51-5 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 941-52-6 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α,4-dimethyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

● HCl

RN 943-23-7 CAPLUS
CN Mandelamidine, N,α-dimethyl-, monohydrochloride, (-)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

L4 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 971-52-8 CAPLUS
CN Mandelic acid, (S)-, compd. with (-)-a-hydroxy-a-methylhydratropamidine (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 53633-24-8
CMF C10 H14 N2 O

Rotation (-).

CM 2

CRN 17199-29-0
CMF C8 H8 O3

Absolute stereochemistry. Rotation (+).

RN 971-53-9 CAPLUS
CN Mandelic acid, (R)-, compd. with (+)-p,a-dimethylmandelamidine (1:1) (8CI) (CA INDEX NAME)

CM 1

CRN 46347-67-5
CMF C10 H14 N2 O

Rotation (+).

L4 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 90-64-2
CMF C8 H8 O3

L4 ANSWER 52 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 611-71-2
CMF C8 H8 O3

Absolute stereochemistry. Rotation (-).

RN 94281-37-5 CAPLUS
CN Mandelamidine, N,a-dimethyl-, hydrochloride (7CI) (CA INDEX NAME)

● HCl

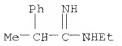
RN 95157-78-1 CAPLUS
CN Mandelic acid, compd. with p,a-dimethylmandelamidine (7CI) (CA INDEX NAME)

CM 1

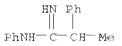
CRN 95157-77-0
CMF C10 H14 N2 O

L4 ANSWER 53 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:475850 CAPLUS
DOCUMENT NUMBER: 57:35850
ORIGINAL REFERENCE NO.: 57:7091i,7092a-d
TITLE: The structure of N-mono- and N,N'-disubstituted amidines
AUTHOR(S): Prevorsek, Dusan C.
CORPORATE SOURCE: Textile Res. Inst., Princeton, NJ
SOURCE: Journal of Physical Chemistry (1962), 66, 763-78
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Factors influencing the position of tautomeric equilibrium of a number of N-mono- and N,N'-disubstituted amidines were studied by infrared spectral analyses. In solution the unsubstituted amidines, RC(:NH)·NH2 .dblarw. RC(:NH)NHR' (I) (R' = H), existed as a mixture of approx. equal amts. of each tautomer. The equilibrium of I was found to be displaced in proportion to the electroneg. of the substituents R'. Thus, when R' was phenyl or hydroxyl (amidoximes), the equilibrium was shifted to a the left, whereas an ethyl group shifted the equilibrium to the right. The nature of the R group apparently was without effect. Characteristic frequency assignments in the 2-7° region for eight N-monosubstituted amidines and seven amidoximes were given where R varied from 2-thienyl, 2-, 3-, or 4-piperidyl, benzyl, a-phenethyl, a-phenylpropyl, and ephenylbutyl groups, R' = H, and R'' = hydroxyl, phenyl, methyl, or ethyl. The spectra of N,N'-disubstituted amidines (II) in dilute solutions showed two bands in the 3 μ region, b suggesting the presence of either two forms of a monomer or a single form giving rise to both bands. Geometric isomerism with respect to the C:N bond was felt unlikely because of the steric effects offered by the R' and R'' groups (substituted phenyl or naphthyl groups). The possibility that one band was an overtone of the fundamental C:N stretching vibration in the 6 μ region was also deemed improbable. Simple tautomerism could not explain the two bands, since identical configurations would result when R' = R''. It was concluded, however, that N,N'-disubstituted amidines very probably exhibited in solution tautomerism leading to a rotational isomerism with respect to both single and double CN bonds. This would explain the appearance of two N-H and C:N bands for derivs. with identical substituents. Characteristic frequency assignments in the 2-7 μ region for ten N,N'disubstituted amidines were given where R = methyl, a-phenethyl, and a-phenylpropyl, R' and (or) R'' = ethyl, phenyl, substituted phenyl, or β-naphthyl The infrared spectra of these N-mono- and N,N'-disubstituted amidines d indicated an electronic configuration similar to that of amides All the amidines studied were prepared according to known procedures.
IT 91429-53-7, Hydratropamidine, N-ethyl- 92579-12-9P, Hydratropamidine, N-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 91429-53-7 CAPLUS
CN Hydratropamidine, N-ethyl- (6CI, 7CI) (CA INDEX NAME)

L4 ANSWER 53 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



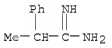
RN 92579-12-9 CAPLUS
CN Hydratropamidine, N-phenyl- (6CI, 7CI) (CA INDEX NAME)



L4 ANSWER 54 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:410679 CAPLUS
DOCUMENT NUMBER: 57:10679
ORIGINAL REFERENCE NO.: 57:2141d-i,2142a-b
TITLE: Amidines and other derivs. of phenylalkylacetic acids
AUTHOR(S): Delaby, Raymond; Reynaud, Pierre; Lilly, Franck
SOURCE: Bulletin de la Societe Chimique de France (1961) 2067
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:10679

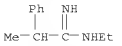
AB Starting with phenylalkylacetonitriles, the title compds. were prepared in order to ascertain their possible hypocholesterolemic action (Redel and Cottet, CA 48, 13061i; C., et al., 13975c). The first step was the preparation of the HCl salt of the imino ester; e.g., PhMeCHC(:NH)OEt.HCl (I) was prepared by passing a current of HCl into a mixture of 20 g. PhMeCHCN (II), 40 cc. Et2O, and 40 cc. absolute EtOH at 0-5° 2.5 hrs. and keeping 2 days at 0°. After removing the solvent in vacuo the residual oil was crystallized from Et2O to yield 92% I, m. 106°; free imino ester (III) b13 116°, n23D 1.5064. PhMeCHC(:NH)NH2.HCl (IV) resulted when 10 g. I in 40 cc. EtOH was treated with NH3 0.5 hr., then refluxed 0.5 hr., the solvent distilled in vacuo, and the residue crystallized from hot H2O; yield, 8.5 g. IV, m. 235°. The following PhCHRC(:NH)OEt.HCl were obtained (R, % yield, m.p., b.p., b.p. pressure (mm.) given): Me, 92,106°,-,-; Et, 87, 98°, -, -; Pr, 83, 82°, -, -. The data for PhCHRC(:NH)OEt were: Me, 82, -, 116°, 13; Et, 84, -, 121°, 15; Pr, 81, -, 103°, 1. The data for PhCHRC(:NH)NH2,HCl were: Me, 98, 235°, -, -; Et, 99, 232°, -, -; Pr, 99, 238°, -,-. Mono- and dialkylamidines were obtained by the action of AlCl3 (V) on a mixture of nitrile and amine. The following PhCHRC(:NH)NR'R''.HCl were prepared (R, R', R'', % yield, b.p./mm., and m.p. given): H, H, Et, 85, 110°/0.1, 61°; H, Et, Et, 68, 131°/2.5, -; H, H, Ph, 95, -, 138°; Me, H, Et, 75, 109°/0.2, -; Me, Et, Et, 62, 111°/0.1, -; Me, H, Ph, 84, -, 89°; Et, H, Et, 99, 115°/0.15, -; Et, Et, Et, 50, -, 45°; Et, H, Ph, 91, -, 86°; Pr, H, Et, 67, 152°/3, -; Pr, Et, Et, 54, 102°/ 0.01, -; Pr, H, Ph, 96, -, 110.5°; n-C8H17, H, Et, 75, 143°/0.1, -; n-C8H17, Et, Et, 53, 160°/0.3, -; n-C8H17, H, Ph, 62, -, 52°. The acids were prepared by saponification of the nitriles. E.g., a solution of 86 g. KOH and 50.3 g. II in 400 cc. EtOH was refluxed 16 hrs. (NH3 evolution was virtually complete in 12 hrs.), the EtOH distilled in vacuo, the residue dissolved in H2O and extracted with Et2O to remove neutral compds. (less than 0.2 g.), the H2O layer acidified, and the free acid extracted from it with Et2O; yield, 89% PhMe-CHCO2H (VI), b13 145°, m. about 16%, n24D 1.5210. VI was

L4 ANSWER 54 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
converted by SOCl2 into 96% PhMeCHCOCI (VII), b13 100-1°. The following PhCHRCO2H and chlorides were prepd. (R, m.p., b.p./mm., and % yield of acid, and b.p./mm. and % yield of chloride given): H, 78°, 144°/12. 92, 95°/14, 88; Me, about 16°, 145°/13, 89, 101°/13, 96; Et, 42°, 158°/15, 85, 112°/16, 97; Pr, 52% 167°/15, 90, 118°/13, 96; n-C8H17, -, 170-3°/0.3, 93, 138°/0.3, 88. The various amides were prepd. from the COCl derivs.; e.g., 8.5 g. VII and 5 g. EtNH2 were each dissolved in 75 cc. C6H6, stirred together, and refluxed 0.5 hr. (1 hr. for the higher homologs). After cooling, EtNH2.HCl was dissolved in H2O, the soln. extd. with Et2O and the ext. added to the C6H5 layer, dried over Na2SO4, and the solvents removed in vacuo. The residue of PhMeCHCONHEt crystd. on cooling; yield after 2 crystns. from C6H6-petr. ether (8:92) 83%, m. 65.5-6°. PhMeCHCONH2 was prepd. similarly, using excess NH3 and not allowing the temp. to exceed 65°; yield 83% after crystn. from C6H6, m. 92.5°. The following PhCHRCONR'R'' were prepd. (R, R', R'' 157°;, H, H, Et, 96, -, 69, 5°; H, Et, Et, 98, 119°/0.3, -; H, H, Ph, 95, -, 113°; H, H, PhCH2, 93, -, 119°; Me, H, H, 89, -, 92.5°; Me, H, Et, 95, -, 66°; Me, Et, Et, 94, 105°/0.15, about 16°; Me, H, Ph, 94, -, 134°; Me, H, PhCH2, 96, -, 75°; Et, H, H, 97, -, 84°; Et, H, Et, 93, -, 66°; Et, Et, 96, 115°/0.2, 32°, 5; Et, H, Ph, 98, -, 97°; Et, H, PhCH2, 93, -, 82°; n-C8H17, H, H, 99, -, 86°; n-C8H17 H, Et, 95, -, 53°; n-C8H17 Et, Et, 98, 168-9°/0.2, -; n-C8H17 H, Ph, 93, -, 66°; n-C8H17 H, PhCH2, 99, -, 52°.
IT 78622-24-9P, Hydratropamidine, hydrochloride 91429-53-7P
, Hydratropamidine, N-ethyl- 92579-12-9P, Hydratropamidine, N-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 78622-24-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



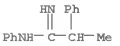
● HCl

RN 91429-53-7 CAPLUS
CN Hydratropamidine, N-ethyl- (6Cl, 7CI) (CA INDEX NAME)



RN 92579-12-9 CAPLUS
CN Hydratropamidine, N-phenyl- (6Cl, 7CI) (CA INDEX NAME)

L4 ANSWER 54 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



L4 ANSWER 55 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:402752 CAPLUS
DOCUMENT NUMBER: 57:7752
ORIGINAL REFERENCE NO.: 57:1128a-c
TITLE: Complexes formed by α-hydroxy amidines with transition metal ions. I. Acid dissociation constants of ligands
AUTHOR(S): Gould, B. C.; Jameson, R. F.
CORPORATE SOURCE: Queen's Coll., Dundee, UK
SOURCE: Journal of the Chemical Society (1962) 294-9
CODEN: JCSOAA; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The first-order rate consts. for the decomposition of (S)-
HOC(Ph)(R)C(:NH)NHBz [R = H (II); R = Me (III)] and S- (R- (III)) at 25G are 18.0 (II), 8.4 (III), and 8.1 (III) × 1-5/sec.; the acid dissociation consts., pK and pK', at 25° are 1, 10.83 ± 0.01 and 12.52 ± 0.05; II, 10.96 ± 0.01 and 12.72 ± 0.05; and III, 11.06 ± 0.01 and 12.86 ± 0.05.
IT 92442-87-0, Mandelanidine, α-methyl-, hydrochloride
(decomposition and ionization of)
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● xHCl

L4 ANSWER 56 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:47579 CAPLUS
DOCUMENT NUMBER: 55:47579
ORIGINAL REFERENCE NO.: 55:9140i,9141a
TITLE: Complexes formed by α-hydroxy amidines with transition metal ions
AUTHOR(S): Gould, B. C.; Jameson, R. F.; Neilson, D. G.
CORPORATE SOURCE: Queen's Coll., Dundee, UK
SOURCE: Proc. Chem. Soc. (1960) 314-15
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Reaction of moist AgIO with PhMeOC(C:NH)NHC) NHC gave an atrolactamidine which could not be freed from Ag. Insertion of α-hydroxy amidines PhXC(OH)C(:NH)NHR (I; X = H, Me, or Et) with Cu++ or Ni++ gave colored complexes. His (mandelamidine)nickel(II), obtained by extraction from aqueous solution with AmCH, was pink and diamagnetic, suggesting the square planar configuration, but the characteristic absorption at 25,000 cm.-1 was absent. Assuming octahedral coordination, if the band at 24,000 cm.-1 was assigned to the 3T1g(F) transition, the 3T2g and 3T1g(F) bands should have been at 13,500 and 34,000 cm.-1 Such bands were observed at 16,000 and 36,000 cm.-1, suggesting octahedral configuration, possibly involving solvent mols. Titration data indicated the mandelamidinium ion is a dibasic acid, pK1 10.5, pK2 12.2.
IT 109595-37-1P, Atrolactamidine, complex with Ni
RL: PREP (Preparation)
(formation of)
RN 109595-37-1 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl- (CA INDEX NAME)

L4 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1959:82995 CAPLUS
DOCUMENT NUMBER: 53:82995
ORIGINAL REFERENCE NO.: 53:14929i,14930a-e
TITLE: Stereochemical structure. XII. Resolution of (±)-atrolactamidinium chloride
AUTHOR(S): Roger, R.; Neilson, D. G.
CORPORATE SOURCE: Queen's Coll., Dundee, UK
SOURCE: Journal of the Chemical Society (1959) 688-90
CODEN: JCSOAA; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 49, 13235e. (±)-Atrolactamidinium chloride (I) was prepared from PhAc cyanohydrin (II) via Et (±)-atrolactimidate·HCl (III).
(±)-Atrolactanidine (IV) was resolved by separation of the diastereoisomeric salts with optically active mandelic acid (V). (-)-Atrolactic acid (VI), isolated from (-)-atrolactamidine chloride (VII), was of at least 90% optical purity. PhMe (120 g.) in 90 ml. Et2O and 123 g. NaCN in 150 ml. H2O treated at 5° during 2 hrs. with 210 ml. concentrated HCl, the Et2O layer separated and the aqueous layer again extracted with Et2O, and the ethereal exts. distilled gave 48 g. II, b18 147-9°, yellow oil. II (48 g.) and 26 g. anhydrous alc. treated 48 hrs. at 0° with 13.2 g. dry HCl and Et2O gave 60 g. III, m. 101-2° (decomposition). III (5 g.) treated with 12 ml. 4N NaOH gave 2 g. Et (±)-atrolactimidate, m. 56-7° (ligroine). An anhydrous solution of 8.5 g. NH3 in 100 ml. alc. shaken 12 hrs. with 23 g. III and the solution evaporated at room temperature gave 17 g. I, m. 174-5° (dilute HCl). I (6 g.) shaken at 0° with 13 ml. 12N NaOH and H2O added gave 3.7 g. IV, m. 75-8° (decomposition); picrate m. 188-9°. I (2.5 g.) heated with 2.2 g. Na salt V in H2O to a clear solution gave 1 g. (+)-atrolactamidine (+)-mandelate (VIII), m. 155-6° (H2O). I (6.7 g.) and 5.8 g. Na (+)-mandelate heated in 37 ml. H2O gave 2 g. (+)-atrolactamidine (+)-mandelate (IX), m. 165° (decomposition), [α]18 +61.3±2° (c 0.91, MeOH). Ethereal (+)-mandelic acid (1.5 g.), [α]7461 186° (MeOH), mixed with 2.6 g. IV in alc. gave 0.7 g. IX. (+)-Atrolactamidine (-)-mandelate (X) was prepared as in the above method but with (-)-mandelic acid. X softened at 162°, m. 165° (decomposition), [α]18 5461 -13.5° (c 0.86, MeOH). IX set aside 24 hrs. with anhydrous HCl-Et2O gave VII, m. 200-1° (decomposition), [α]18 5461 -55.6° (c 0.54, H2O). Similarly X yielded (-)-atrolactamidinium chloride, softened at 178°, m. 202° (decomposition), [α]18 5461 (c 0.58, H2O); the yield was almost theoretical. VII (0.5 g.) heated in 6N NaOH until evolution of NH3 ceased, the solution acidified, and extracted with Et2O gave 0.2 g. VI, [α]22D -48.3° (c 0.55, H2O). The 2 forms of I treated at 0° with alkaline solns. of varying strengths did not give crystalline products. The rotatory powers of the optically active forms of I at 3 wavelengths in the visible spectrum gave approx. straight line Lowry-Dickson plots but the detns. were not sufficient to warrant discussion.
IT 92442-87-0 109595-38-2
(Derived from data in the 6th Collective Formula Index (1957-1961))

L4 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● xHCl

RN 109595-38-2 CAPLUS
CN Mandelic acid, salt with atrolactamidine (6CI) (CA INDEX NAME)

CM 1

CRN 109595-37-1
CMF C9 H12 N2 O

CM 2

CRN 90-64-2
CMF C8 H8 O3

IT 109595-37-1, Atrolactamidine, (-)-
(and derivs.)
RN 109595-37-1 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl- (CA INDEX NAME)

L4 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L4 ANSWER 58 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1959:82994 CAPLUS
DOCUMENT NUMBER: 53:82994
ORIGINAL REFERENCE NO.: 53:14929h
TITLE: Thermal oxidation of methyl esters of fatty acids
AUTHOR(S): Ramanathan, Venkatachalam
CORPORATE SOURCE: Univ. of Illinois, Urbana
SOURCE: (1959) 95 pp. Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 59-564
From: Dissertation Abstr. 19, 2967-8
DOCUMENT TYPE: Dissertation
LANGUAGE: Unavailable
AB Unavailable
IT 92442-87-0 109595-38-2
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 92442-87-0 CAPLUS
CN Benzeneethanimidamide, α-hydroxy-α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● xCl

RN 109595-38-2 CAPLUS
CN Mandelic acid, salt with strolactamidine (6CI) (CA INDEX NAME)

CM 1

CRN 109595-37-1
CMF C9 H12 N2 O

CM 2

CRN 90-64-2
CMF C8 H8 O3

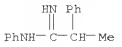
L4 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L4 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:113428 CAPLUS
DOCUMENT NUMBER: 52:113428
ORIGINAL REFERENCE NO.: 52:20024g-i,20025a
TITLE: Research on hypocholesterol. Synthesis of amidines from substituted phenylacetic acids
AUTHOR(S): Delaby, Raymond; Reynaud, Pierre; Lilly, Frank
SOURCE: Compt. rend. (1958), 246, 2905-8
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB PhCH2CN with EtZCO3 in the presence of EtONa gives Et α-cyanophenylacetate, converted by treatment with alkyl halides (RX) and saponification with NaOH to PhCHRCN, e.g. 62% PhCHMeCN, b15 108°, 69% PhCHEtCN, b15 115° 72% PhCHPrCN, b14 130°, and 63% PhCH(CH2CH2-n)CN, b0.1 133°. On passing dry HCl into solns. of the nitriles in EtOH, the iminoesters are formed, and addition of amines in the presence of AlCl3 gives N-substituted amidines. Thus, PhCHMeCN with HCl and EtOH gives PhCHMeC(:NH)OEt.HCl, m. 103.5°, and then PhCHMeC(:NH)NH2.HCl, m. 235°, is ethylated to PhCHMeC(:NH)NHEt, b0.2 105°, and PhCHMeC(:NH)NHEt2, b0.1 111°, or phenylated to PhCHMeC(:NH)NHPh, m. 89°. Similarly, PhCHEtCN gives PhCHEtC(:NH)OEt.HCl, m. 98° then PhCHEtC(:NH)NH2.HCl, 232°, PhCHEtC(:NH)NHEt, b0.15 115°, or PhCHEtC(:NH)NHEt2, m. 45°, and PhCHEtC(:NH)NHPh, m. 86°. Also, PhCHPrCN gives PhCHPrC(:NH)OEt.HCl, m. 82°, then PhCHPrC(:NH)NH2.HCl, m. 238°, PhCHPrC(:NH)NHEt, b0 152°, or PhCHPrC(:NH)NHEt2, b0.1 102° and PhCHPrC(:NH)NHPh, m. 110.5°. PhCH(CH2CH2-n)CN gives the amidines PhCH(CH2CH2-n)C(:NH)NHEt2, b0.3 160°, and PhCH(CH2CH2-n)-C(:NH)NHPh, m. 52°. The physiol. activity of the substituted amidines is being studied.
IT 78622-24-9P, Hydratropamidine, hydrochloride 91429-53-7P , Hydratropamidine, N-ethyl- 92579-12-9P, Hydratropanidine, N-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 78622-24-9 CAPLUS
CN Benzeneethanimidamide, α-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● xCl

RN 91429-53-7 CAPLUS
CN Hydratropanidine, N-ethyl- (6CI, 7CI) (CA INDEX NAME)

L4 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 92579-12-9 CAPLUS
CN Hydratropamidine, N-phenyl- (6CI, 7CI) (CA INDEX NAME)



L4 ANSWER 60 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1949:38809 CAPLUS
DOCUMENT NUMBER: 43:38809
ORIGINAL REFERENCE NO.: 43:6993c-i,6994a-b
TITLE: Aliphatic nitro compounds. XIX. Friedel-Crafts reactions with α- and β-nitro olefins
AUTHOR(S): Lambert, A.; Rose, J. D.; Weedon, B. C. L.
SOURCE: Journal of the Chemical Society (1949) 42-6
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 42, 4917e. CH2:CMeCH2NO2 (I) (10 g.), added (15 min.) to 16 g. AlCl3 in 50 cc. C6H6 at 30°, stirred 1 hr. at 30-40°, and poured onto concentrated HCl and ice, gives 9.55 g. 1-nitro-2-phenyl-2-methylpropane (II), b0.1 67-70°, nD23 1.5235; II results in 13-g. yield from PhMgBr (9.6 g. Mg) in 300 cc. ether on addition (1.5 hrs.) to 40 g. Me2C:CHNO2 in 300 cc. H2O at -5 to 0°, refluxing 0.5 hr., and decomposing with 24 g. AcOH in 160 cc. H2O. Reduction of 4 g. II in 50 cc. MeOH over Raney Ni at room temperature and atmospheric pressure gives 2.5 g. 2-phenyl-2-methylpropylamine, b14 96-8° (picrate, yellow, m. 160°). I (10 g.) in 100 cc. PhMe, saturated with BF3, kept at room temperature overnight, and heated 1 hr. at 70-80°, gives 5 g. 1-nitro-2-p-tolyl-2-methylpropane (III), pale yellow, b0.5 85-90°, b13 145-50°, nD22 1.5258. III (0.4 g.), boiled 4 hrs. with 3 g. KMnO4 in 25 cc. H2O, gives 0.3 g. α,α-dimethylhomoterephthalic acid (IV), m. 236-7°. Catalytic reduction (as above) of 3.6 g. III yields 2.5 g. 2-p-tolyl-2-methylpropylamine, b10 111.5-15°, b32 134°, nD22 1.5231 (picrate, yellow, m. 211-13°). Me2C:CHNO2 (20 g.) in 100 cc. PhMe, saturated with BF3 at 50°, gives 8.5 g. α-(p-tolyl)isobutyrohydroxamic acid (V), m. 157°, gives a deep red-violet color with FeCl3, and reduces AgNO3 in NH4OH. Distillation of the residue from the PhMe yields 6 g. III and a small quantity of a compound (C11H13ON ?), m. 132-4°. Catalytic reduction of 0.9 g. V in MeOH yields 0.5 g. α-(p-tolyl)isobutyramide (VI), m. 143-4°. VI (0.2 g.) and 15 cc. 2 N HCl, refluxed 10 hrs., give 0.17 g. α-(p-tolyl)isobutyric acid (VII), m. 82°; VII results also on refluxing 0.5 g. V and 15 cc. 2 N HCl 0.5 hr. The structures of the VII reported by Wallach [Nachr. Ges. Wiss. Gottingen 2, 4(1899)] and by Rupe and Burgin (C.A. 5, 2841) are not clear. The Na derivative from 98 g. p-MeC6H4CH2CN (prepared with NaNH2), treated dropwise with 213 g. MeI (1 hr.), gives 42% α-(p-tolyl)isobutyronitrile, b12 122-3°, b763 246°, nD22 1.5106, d2222 0.9661; hydrolysis with KOH yields VI and VII. Oxidation of 4 g. VII in 40 cc. 5% Na2CO3 with 240 cc. 4% KMnO4 (1 hr.) gives 4 g. IV; further oxidation gives p-C6H4(CO2H)2. Details are given of the attempted preparation of VII by the method of R. and B. Me2C:CHNO2 and C6H6 do not yield a hydroxamic acid with BF3. Me2C:CHNO2 (60 g.), added (1 hr.) to 80 g. AlCl3 in 300 cc. C6H6 at 40°, the mixture stirred an addnl. hr., decomposed with HCl and ice, and extracted with C6H6, gives 25 g. α,β-dichloroisobutyraldoxime, Me2CClCCl:NOH,

L4 ANSWER 60 OF 60 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
b14 81-5°, nD25 1.4922, and 22 g. α-phenylisobutyrohydroxamyl chloride (VIII), Me2PhCCCl:NOH, m. 73-4°. VIII and PhNH2 in EtOH give α-phenylisobutyrohydroxamanilide, m. 171-2°. VIII (5 g.) and 2.1 g. NaHCO3 in 100 cc. H2O, shaken 0.5 hr., give 2 g. 1-phenylisopropyl isocyanate (IX), b0.16 50-2°, nD22 1.5038; with PhNH2 it yields 1-phenyl-3-(1-phenylisopropyl)urea, m. 193-4°. IX (0.6 g.), refluxed 3 hrs. with aq. NaHCO3, gives 0.4 g. 1,3-bis(1-phenylisopropyl)urea, (PhMe2CNH)2CO, m. 226-7°. Hydrogenation of 4 g. of IX over Raney Ni gives 1.6 g. 1-methyl-1,3-bis(1-phenylisopropyl)urea, PhMe2CNMeCONHC-PhMe2, m. 171-2°. MeCH(OH)CHNO2 (50 g.), C6H6, and AlCl3, refluxed 4 hrs., give 23% PhCH:NOH and 9 g. MeCHPh2; this can be explained by the initial formation of MeNO2 and MeCHO. MeNO2 and C6H6 give PhCH:NOH and PhN:CHPh.
IT 858208-39-6P, Hydratropanilide, α-methyl-, oxime
RL: PREP (Preparation)
(preparation of)
RN 858208-39-6 CAPLUS
CN Benzeneethanimidamide, N-hydroxy-α,α-dimethyl-N'-phenyl- (CA INDEX NAME)